# FlexFL: Flexible and Effective Fault Localization with Open-Source Large Language Models

Chuyang Xu, Zhongxin Liu, Xiaoxue Ren, Gehao Zhang, Ming Liang, David Lo

Abstract—Fault localization (FL) targets identifying bug locations within a software system, which can enhance debugging efficiency and improve software quality. Due to the impressive code comprehension ability of Large Language Models (LLMs), a few studies have proposed to leverage LLMs to locate bugs, i.e., LLM-based FL, and demonstrated promising performance. However, first, these methods are limited in flexibility. They rely on bug-triggering test cases to perform FL and cannot make use of other available bug-related information, e.g., bug reports. Second, they are built upon proprietary LLMs, which are, although powerful, confronted with risks in data privacy. To address these limitations, we propose a novel LLM-based FL framework named FlexFL, which can flexibly leverage different types of bug-related information and effectively work with open-source LLMs. FlexFL is composed of two stages. In the first stage, FlexFL reduces the search space of buggy code using state-of-the-art FL techniques of different families and provides a candidate list of bug-related methods. In the second stage, FlexFL leverages LLMs to delve deeper to double-check the code snippets of methods suggested by the first stage and refine fault localization results. In each stage, FlexFL constructs agents based on open-source LLMs, which share the same pipeline that does not postulate any type of bug-related information and can interact with function calls without the out-of-the-box capability. Extensive experimental results on Defects4J demonstrate that FlexFL outperforms the baselines and can work with different open-source LLMs. Specifically, FlexFL with a lightweight open-source LLM Llama3-8B can locate 42 and 63 more bugs than two state-of-the-art LLM-based FL approaches AutoFL and AgentFL that both use GPT-3.5. In addition, FlexFL can localize 93 bugs that cannot be localized by non-LLM-based FL techniques at the top 1. Furthermore, to mitigate potential data contamination, we conduct experiments on a subset of the GHRB dataset that Llama3-8B has not seen before, and the evaluation results show that FlexFL achieves comparable performance on the two datasets.

Index 1	<b>Ferms</b> —Faul	lt Localization, I	Large Languag	ge Model, LLM-b	ased Agent	

#### 1 Introduction

Fault localization (FL) is tasked with precisely identifying the locations of bugs within a software system [1]. Effective FL can significantly enhance the efficiency of debugging by concentrating on the buggy areas, improving software quality and developer productivity [2]. To facilitate debugging, prior work has proposed many approaches to automatically localize buggy program entities (e.g., statements, methods, and files), among which information-retrieval-based techniques (IRFL) [3]–[6], spectrum-based techniques (SBFL) [7]–[10] and hybrid fault localization (HybridFL) [11], [12] have shown to be effective.

Recently, due to the capability of large language models (LLMs) in language understanding, planning, and reasoning [13]–[21], LLMs have attracted significant attention from software debugging researchers with successful research done on patch generation [22] and bug reproduction [23]. These researches show that LLMs can effectively understand source code and bug-related information (e.g., failed tests), plan the debugging process, and reason the root causes of

 Chuyang Xu, Zhongxin Liu and Xiaoxue Ren are with the State Key Laboratory of Blockchain and Data Security, Zhejiang University, Hangzhou, 310027, China.
 E-mail: {chuyangxu, liu\_zx, xxren}@zju.edu.cn

Gehao Zhang and Ming Liang are with Ant Group, China.
 Email: gehaozhang1999@gmail.com, liangming.liang@antgroup.com

bugs, and thus can be beneficial for FL. A few studies [24]-[27] proposed to automate FL with LLMs. Wu et al. [24] leverage GPT-3.5 and GPT-4 to localize buggy statements in the context of their belonging method or class. However, it is difficult to use as a standalone FL technique in practice because locating faulty methods or classes remains a difficult problem for existing FL techniques. AgentFL [26] and AutoFL [25] focus on localizing the buggy methods from an entire project, which are more practical and achieve promising results. AgentFL [26] starts with bug-triggering test cases (for short, trigger tests) and leverages a manually crafted and fixed procedure to iteratively prompt ChatGPT to identify buggy locations. Kang et al. [25] proposed AutoFL that equips GPT3.5 and GPT-4 with function calls (i.e., external tools or programs provided by users) to get the classes and methods covered by trigger tests and access the actual code snippets in the project, achieving state-of-the-art performance.

LLM-based FL techniques [25], [26] have outperformed traditional non-LLM-based FL techniques. However, they have the following limitations. (1) Their flexibility in handling different types of bug-related information is limited. AgentFL and AutoFL both rely on trigger tests to build pipelines or agents. Therefore, them can only work when trigger tests are available and cannot leverage other bug-related information, e.g., bug reports. However, in practice, the available bug-related information for different bugs may differ. For example, only bug-triggering test cases are available for the bugs found by fuzzing tools, while the bugs reported by users may only have bug reports

David Lo is with the School of Computing and Information Systems, Singapore Management University, Singapore 188065
 E-mail: davidlo@smu.edu.sg

<sup>•</sup> Zhongxin Liu is the corresponding author.

for FL. Furthermore, leveraging all available bug-related information can improve FL performance [11], [12]. (2) They are based on closed-source LLMs, which are confronted with concerns about data privacy. Existing LLMbased FL techniques [24]-[26] all leverage GPT-3.5 or even GPT-4, which have demonstrated powerful capacities for instruction compliance and task solving. It is still unknown whether they can work with open-source LLMs, which are widely used by organizations concerned with data privacy but have limited context length and inferior performance. In addition, AutoFL [25] leverages the out-of-the-box function calling capability of OpenAI GPT<sup>1</sup>. This capability enables users to merely provide function descriptions for the GPT, which can accurately respond with a complete function call with arguments in the JSON format. To the best of our knowledge, this capability is not provided by most opensource LLMs.

To fill these gaps, we propose a novel LLM-based FL framework FlexFL, which can flexibly leverage different types of bug-related information to localize buggy methods with open-source LLMs effectively. Specifically, FlexFL comprises two stages: ① space reduction and ② localization refinement. In the first stage, FlexFL utilizes an LLM-based agent named Agent4SR and non-LLM-based FL approaches to produce a candidate list of methods related to bugs. In the second stage, FlexFL constructs another agent named Agent4LR to refine the locations predicted in the space reduction stage by focusing on double-checking the code snippets of the predicted locations.

The differences between FlexFL and existing LLM-based FL techniques [25], [26] are as follows: First, the two LLMbased agents in FlexFL are designed to share the same pipeline that does not postulate any type of bug-related information, ensuring the flexibility of FlexFL. Second, FlexFL combines LLM-based agents and non-LLM-based FL approaches in the first stage. FlexFL uses existing non-LLMbased FL techniques regardless of how they work to localize bugs and thus can process any input they can handle, benefiting FlexFL's flexibility. In addition, non-LLM-based FL techniques [6], [7], [11] are proven helpful to filter out methods unrelated to bugs and thus can effectively reduce search space for FlexFL. Third, FlexFL adopts a two-stage process. After space reduction in the first stage, LLM-based agents in the second stage can fully leverage LLMs' capabilities for code comprehension and reasoning to focus on checking the code snippets of the most suspicious methods. This design mitigates the impact of the limited context length of LLMs and their inferior performance on long input contexts [28], which is more severe for opensource LLMs, and thus enables effective fault localization with open-source LLMs. Fourth, we utilize open-source LLMs to construct two LLM-based agents, i.e., Agent4SR and Agent4LR. It is non-trivial to build them upon opensource LLMs since they do not provide the out-of-thebox function calling capability, which can effectively assist LLMs in using external tools. Inspired by the reason-andact paradigm [19], we first prompt open-source LLMs to fully reason and plan how to act based on available bugrelated information. Then, we instruct open-source LLMs to

1. https://platform.openai.com/docs/guides/gpt/function-calling

call functions (i.e., external tools) in the right format, which helps automate their interactions with provided function calls. In addition, open-source LLMs usually suffer more from hallucination [29] and long input contexts, and thus often generate inaccurate names of program entities even though these have been mentioned in the context, preventing LLMs from performing follow-up actions efficiently. To tackle this problem, we propose a postprocessing process to effectively match inaccurate names to actual program entities in the buggy program through fuzzy search.

We perform thorough experiments to evaluate the effectiveness of FlexFL and the contributions of its components. We evaluate FlexFL on a widely used debugging benchmark Defects4J [30]. Experimental results show that FlexFL outperforms non-LLM-based FL baselines and the LLM-based techniques that use GPT-3.5 in all metrics. For example, FlexFL with Llama3-8B-Instruct [16], a lightweight open-source LLM, can localize 12.3%, 18.9%, 21.6% more bugs than the state-of-the-art LLM-based approach AutoFL with GPT-3.5, in top-1, top-3, and top-5, respectively. We also implement FlexFL based on two other lightweight open-source LLMs, i.e., Qwen2-7B-Instruct [17] and Mistral-Nemo-12B-Instruct [31], of which the comparable performance indicates FlexFL is generalizable across different lightweight open-source LLMs. To investigate the impact of potential data leakage of LLMs, we evaluate FlexFL on 38 recently fixed bugs from the GHRB [32] dataset, where the performance of FlexFL is close to its performance on the Defects4J dataset. These experimental results show that FlexFL achieves flexible and effective fault localization based on open-source LLMs.

In summary, we make the following contributions.

- We propose a flexible and effective fault localization framework named FlexFL, which can handle different types of bug-related information and is effective.
- We enable the construction of agents based on opensource LLMs for FL. To the best of our knowledge, this is the first attempt to build FL agents based on opensource LLMs.
- We comprehensively evaluate FlexFL, and evaluation results show that our framework outperforms the baselines by substantial margins.
- We open source our replication package [33], including the dataset, the source code of FlexFL, and experimental results, for follow-up works.

The remainder of the paper is organized as follows. Section 2 gives an overview of the relevant literature, and Section 3 describes our approach. Evaluation settings and research questions are in Section 4. Results are presented in Section 5, while threats to validity are in Section 6. Section 7 concludes and describes future work..

# 2 BACKGROUND AND RELATED WORK

Our framework FlexFL focuses on method-level FL, i.e., locating buggy methods from an entire project. In this section, we review existing non-LLM-based FL techniques and then introduce the related LLM-based FL techniques.

#### 2.1 Non-LLM-based Fault Localization

Typical method-level FL techniques include Spectrum-based Fault Localization (SBFL), Information Retrieval-based Fault Localization (IRFL), Mutation-based Fault Localization (MBFL), and Hybrid Fault Localization (HybridFL), which combines two or more FL techniques.

Information Retrieval-based Fault Localization (IRFL) [34] measures the textual similarity between bug reports and program entities, and outputs a ranked list of program entities as suspicious bug locations. To the best of our knowledge, only a few IRFL techniques can localize bugs at the method level [4]–[6], [35]. Among them, BoostNSift [6] achieves the state-of-the-art method-level FL performance by embedding query boosting and code sifting in conjunction with the BM25 Information Retrieval (IR) model. In the query boosting step, BoostNSift adds weights to the title field of the bug report. In code sifting, the relevance of a program entity to a specific bug report is compared against its relevance to a collection of bug

Spectrum-based Fault Localization (SBFL) is one of the most prevalent fault localization techniques [2], which are broadly adopted in program debugging [7], [11]. SBFL techniques analyze the run-time behavior of the passing and failing test cases and rank program entities based on program spectrum [2]. Traditional formula-based SBFL techniques calculate suspiciousness scores using a ranking metric, e.g., Ochiai [7], Dstar [8], and Tarantula [36].

Mutation-based Fault Localization (MBFL) [37] injects changes to each program entity (based on mutation testing [38]) to check its impact on the test outcomes. Different from SBFL techniques, which consider whether a statement is executed or not, MBFL techniques [39]–[41] consider whether the execution of a statement affects the result of a test by injecting mutants. The more often a statement affects failing tests, and the less often it affects passing tests, the more suspicious the statement is considered. For a statement s, an MBFL technique generates a set of mutants mut(s), assigns each mutant a score M(m), and aggregates the M(m) to yield a statement suspiciousness score S(s). MUSE [39] and Metallaxis-FL [40] are two state-of-the-art MBFL techniques, both of which use different formulas to calculate M(m) and different strategies for aggregation.

Hybrid Fault Localization (HybridFL) [2], [11] combines results of different FL techniques. CombineFL [2], DeepFL [42], and FLUCCS [43] use learning-to-rank [44] machine learning approaches such as RankSVM [45] to combine multiple FL techniques, which need additional datasets for training. SBIR [11] uses the Monte Carlo rank aggregation algorithm [46] to combine IRFL and SBFL techniques' ranked lists, which is an unsupervised HybridFL approach and achieves state-of-the-art performance.

#### 2.2 LLM-based Fault Localization

Large language models (LLMs) have shown remarkable effectiveness in solving complex software engineering problems [23], [47]–[49]. This success has drawn some attention from the fault localization research community [24]–[27]. Specifically, Wu et al. [24] have assessed the effectiveness using GPT-3.5 and GPT-4 in locating buggy statements from

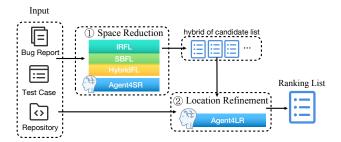


Fig. 1. The Overall Framework of FlexFL

a given code snippet, e.g., a buggy class or a buggy method. Different from Wu et al.'s work, our work focuses on method-level FL and does not assume a known buggy code snippet. AutoFL [25] starts from the classes and methods covered by failing test cases and leverages the function-calling capability of GPT-3.5 and GPT-4 to inspect code and pinpoint buggy methods from a project. AgentFL [26] takes failing test cases as input and prompts ChatGPT multiple times with diversified information to handle manually designed tasks in each step of its process. Different from AutoFL and AgentFL, our approach is more flexible, can take as input different types of bug-related information, and can effectively work with open-source LLMs.

# 3 METHODOLOGY

We propose FlexFL, a flexible and effective LLM-powered framework for method-level fault localization. This section first introduces the overall framework of FlexFL, then describes the design of two agents in FlexFL (i.e., Agent4SR and Agent4LR).

#### 3.1 Overview of FlexFL

Figure 1 shows the overall framework of our FlexFL. Given the repository containing the bug and available bug-related information, e.g., the bug report or/and test cases, FlexFL produces a ranking list of the top k most suspicious methods responsible for the bug. Specifically, FlexFL contains two stages ① space reduction and ② localization refinement. In the first stage, FlexFL utilizes an LLM-based agent named Agent4SR and non-LLM-based FL approaches, e.g., IRFL, SBFL, and HybridFL techniques, to obtain a hybrid of candidate list that contains m suspicious methods. In the second stage, FlexFL leverages another LLM-based agent named Agent4LR to double-check the code snippets of the suggested methods in the candidate list and localize the top-k most suspicious methods. The design of the two-stage process can help fully leverage LLMs' powerful capacity in language understanding and reasoning to focus on the most suspicious methods, enabling effective fault localization.

#### 3.1.1 Input of FlexFL

Our FlexFL incorporates two flexible types of bug-related information, i.e., bug reports and test suites, as input, while existing LLM-based FL techniques [25], [26] can only leverage bug-triggering test cases (for short, trigger tests) in test suites. Following these studies, we input trigger tests to LLMs in text, which contains the

TABLE 1
Text Description of Input(Example Bug: Time-25 in Defects4J [30])

Bug Report	Title: #90 DateTimeZone.getOffsetFromLocal error during DST transition  Description: This may be a failure of my understanding, but the comments in DateTimeZone.getOffsetFromLocal lead me to believe that if an ambiguous local time is given, the offset corresponding to the later of the two possible UTC instants will be returned - i.e. the greater offset(More details in [50])
Trigger Test	public void test_DateTime_constructor_Moscow_Autumn() {     DateTime dt = new DateTime(2007, 10, 28, 2, 30, ZONE_MOSCOW);     assertEquals("2007-10-28T02:30:00.000+04:00", dt.toString());     The last line shown above failed with the following stack trace.     junit.framework.ComparisonFailure: expected:<10-28T02:30:00.000+0[4]:00> but was:<10-28T02:30:00.000+0[3]:00>     at junit.framework.Assert.assertEquals(Assert.java:100)     at org.joda.time.TestDateTimeZoneCutover.test_DateTime_constructor_Moscow_Autumn(TestDateTimeZoneCutover.java:922)

test methods and their stack traces. As shown in Table 1, we remove the methods that do not belong to the buggy program (e.g., at junit.framework.Assert. assertEquals(Assert.java:100)) from the stack trace, and truncate the test method at the point of failure to highlight critical information and save context length. For bug reports, which are neglected by previous LLM-based works, we construct the text descriptions in the format shown in Table 1, which explicitly points out the titles and descriptions. Note that these inputs (i.e., bug reports and trigger tests) can be processed not only individually but also in combination by LLMs via a dynamic prompt, offering FlexFL the flexibility in addressing various fault localization scenarios. For non-LLM-based FL approaches, these two types of bug-related information are input in the suitable ways they require. Specifically, bug reports are also used in their text form for lexical match in IRFL techniques, and test suites are executed for collecting dynamic execution information (e.g., program spectrum) in SBFL techniques.

A critical input for FL tasks is the entire software repository containing the bug. However, it is costly and ineffective to directly feed the whole large program into LLMs for processing since the computational complexity of existing LLMs is quadratic and the performance of LLMs degrades as the length of input contexts increases [28]. To solve this problem, the prior work AutoFL [25] allows LLMs to navigate the source code by calling custom-designed functions that return the information of the classes and methods covered by trigger tests, and access the implementation and documentation of any covered method. Inspired by AutoFL, we also designed a set of custom-designed function calls for LLMs to enable code exploration and relevant information extraction from the buggy program. However, different from AutoFL where the designed function calls require coverage information collected with trigger tests, our designed function calls do not rely on any type of bugrelated information and thus ensure the flexibility of FlexFL.

#### 3.1.2 Space Reduction

This stage aims to effectively narrow down the search space before localizing the buggy methods based on the constructed input. Previous studies [25], [26] have shown that LLM-based agents can automatically search for bugrelated methods over a large software repository, which can be beneficial for reducing the search space. Therefore, we design an agent named Agent4SR based on open-source LLMs, which aims to reduce the bug-related code space via

global searching in the buggy program. In addition, existing non-LLM-based FL techniques have been proven helpful and valuable for filtering out unrelated methods in the buggy program [2], [6], [7], [11], [39]. Based on this idea, we propose to combine Agent4SR with existing non-LLM-based FL techniques to complement Agent4SR and better reduce the search space. Specifically, given input introduced in Section 3.1.1, Agent4SR and non-LLM-based FL techniques respectively localize the top-k most suspicious methods responsible for the bug. To combine the suggested methods of Agent4SR and non-LLM-based FL techniques, we first place the results of Agent4SR (i.e., top-k buggy methods) at the end based on the assumption that the methods localized by Agent4SR are more likely to be localized by Agent4LR, which is also an LLM-based agent, so we do not need to emphasize them via high ranking. Then, the remaining  $m\!-\!k$ methods are divided equally among the non-LLM-based FL techniques and the top-k results of one technique would be followed by the top-k results of another. The order of non-LLM-based FL techniques is based on another assumption that more precise localization results should be assigned a higher ranking to assist LLMs in refinement. Finally, after space reduction, we can obtain a relatively comprehensive candidate list that contains m suspicious methods. These methods are localized by different techniques in various ways, thus containing diverse kinds of information beneficial for localization refinement. For instance, Agent4SR focuses on the semantic information extracted from the textual description of trigger tests while SBFL approaches emphasize dynamic execution information of test suites.

In this stage, FlexFL employs existing non-LLM-based FL techniques and thus is enabled to process any type of input that previous approaches can handle.

#### 3.1.3 Localization Refinement

For localization refinement, we further design an agent, named Agent4LR, which localizes the top-k most suspicious methods based on the textual description of bug-related information and the candidate list produced in the space reduction stage. Unlike Agent4SR, Agent4LR is aimed at double-checking the suspicious methods in the candidate list. This design enables Agent4LR to use more tokens for planning, reasoning, and understanding, instead of code exploration, thus alleviating LLMs' limitation in processing long context. More details can be found in Section 3.2.5.

# 3.2 Design of Agents

The LLM-based agents within our FlexFL, i.e., Agent4SR and Agent4LR, are constructed following the same pipeline based on open-source LLMs. Below, we first outline the overall pipeline of these agents and the function calls designed to assist them. Then, we respectively introduce the detailed designs of Agent4SR and Agent4LR.

# 3.2.1 Pipeline of agents

To prompt open-source LLMs to localize bugs with bugrelated information, both agents in FlexFL are designed to follow a three-step process: task assignment, interaction with function calls, and summarization. Figure 2 uses the bug Time-25 [50] from Table 1 as an example to illustrate this pipeline in detail.

Step 1: Task assignment. In this step, we make agents in FlexFL flexibly handle bug reports and test cases both separately and together via the dynamic prompt. Specifically, we design two prompts containing bug-related information and descriptions of available function calls. The first prompt is a system prompt, as shown in Figure 2, which guides LLMs in their roles as debugging assistants. The task assigned to LLMs is to localize the top k most suspicious methods based on the available bug-related information and the information extracted from the buggy programs via function calls (see Section 3.2.2). Note that if any type of bug-related information is not available, contents relative to it will be deleted from this prompt. For instance, when only bug reports are available, we will instruct the agent to *localize* the top-k most suspicious methods based on the bug report and the information you retrieve in the system prompt that is different from that shown in Figure 2. The second prompt presents the descriptions of available inputs to the agent. For both agents, text descriptions of bug reports and trigger tests (see Table 1) are given in order if available. The candidate list of suggested methods that is an additional type of input for Agent4LR will be placed after descriptions of bug-related information.

**Step 2: Interaction with function calls.** In this step, we design a pipeline for LLMs to interact with function calls via prompt engineering and a postprocessing process, which can assist any chat model in code exploration of software repositories, including lightweight open-source LLMs that do not support the out-of-the-box function calling capability.

Following the insights from ReAct [19], we first prompt LLMs to reason and plan how to use function calls to help LLMs organize their thoughts and develop a strategy for localizing buggy methods, as shown in Figure 2. Through reasoning, the LLMs can form a clear hypothesis about where the bug might be and why it is happening. This prepares them for interaction with function calls, where they can act on these hypotheses to gather more specific information or confirm their hypotheses. For example, the reasoning results of Time-25 show its root cause, i.e., The bug is related to the DateTimeZone.getOffsetFromLocal method, which is responsible for calculating the offset from local time to UTC.

After reasoning, LLMs are prompted to interact with function calls that assist in extracting detailed information from the buggy programs. Different from proprietary LLMs like OpenAI GPT, open-source LLMs do not have

the capability of function calling and cannot accurately identify the function calls needed to be called and precisely construct their arguments. To enable function calling based on open-source LLMs for FL, we first design a prompt that asks LLMs to call a function in the format 'Function-Name(Argument)' in a single line without any other word. Then we process the function call provided by LLMs, e.g., find\_class("DateTimeZone") shown in Figure 2, via the regular expressions that are consistent with the required format. After obtaining the name (e.g. find\_class) and arguments (e.g. "DateTimeZone") of the function call, we match the name and call the corresponding function with the arguments to extract information from the buggy program. Finally, we append the extracted information (e.g., org.joda.time.DateTimeZone in Table 1) to the context and enter the next loop. If the name of the function call provided by LLMs is not included in the given set, we return a prompt Please call functions in the right format 'FunctionName(Argument).'.

Such a conversation will loop *MAX* times, which is also specified in the system prompt. If the whole conversation exceeds the maximum context length of the used LLM, we decrease the value of *MAX* by 1 and rerun this pipeline. In addition, to conserve time and computational resources and further prevent exceeding the context length limit of LLM, we design a fixed and special function call <code>exit()</code>, which does not return information and is provided for LLMs to exit the step of interaction with function calls when LLMs are confident to localize buggy methods. Therefore, this iterative process of information gathering and analysis continues until either the LLMs have performed *MAX* function calls or issued an <code>exit</code> command. This structured interaction ensures that the LLMs gather comprehensive information necessary for precise bug identification.

**Step 3: Summarization.** In this step, we instruct LLMs to summarize and pinpoint the top k most suspicious methods via integrating inputs from Step 1 and the information retrieved in Step 2. To ensure full automation and standardization, the responses from the LLMs are formatted according to a predetermined schema, i.e., *Top\_i: PathName.ClassName.MethodName( ArgTypeList )*, as shown in Figure 2. LLMs cannot always generate accurate names of the code elements even if they have been provided in Step 2. This issue is more common for open-source LLMs. Therefore, the structured output of LLMs will be further refined using our postprocessing process, which matches the method names provided by LLMs to actual methods in the buggy program (see Section 3.2.3). At last, the result is a refined and realistic list of probable buggy methods.

# 3.2.2 Design of Function Calls

We design a set of function calls for the agents in FlexFL to interact with, which assist LLMs in obtaining information related to bugs in the program. These function calls need to know the structure and existing entities of the buggy program. To meet this requirement, we traverse all the files in the program and extract the code snippets of all the methods using a parser. For each method in the program, we record its fully qualified name, which contains its file path, class name, method name, and method signature.

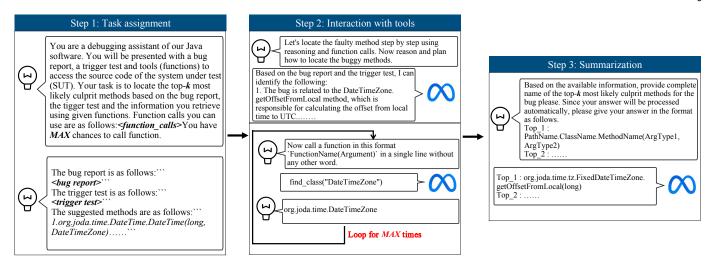


Fig. 2. The pipeline of agents. Bold text in <> indicates placeholders for input contents or description of function calls designed in Section 3.2.2

TABLE 2
Function calls designed for agents

Name	Arguments	Description
get_paths	None	Get the paths of the Java software system
get_classes_of_path	path_name	Get the classes in the path of the Java software system
get_methods_of_class	class_name	Get the methods belonging to the class of the Java software system
get_code_snippet_of_method	method_name	Get the code snippet of the Java method
find_class	class_name	Find the class through fuzzy search
find_method	method_name	Find the method through fuzzy search
exit	None	Exit function calling

We design seven function calls, which are listed and described in Table 2. The function calls beginning with get are intended to enable LLMs to navigate the file structure of the program or retrieve the code snippet of any specified method. They require fully qualified names (FQNs) of corresponding code elements as arguments. However, LLMs often provide inaccurate or incomplete code entity names due to hallucinations [29], [51] and limited capacity, which are more severe for open-source LLMs. For instance, when calling function get\_code\_snippet\_of\_method, LLMs may only provide the name of the function without a signature or its belonging class, like getOffsetFromLocal shown in Table 5, which is incomplete to be precisely paired to any code snippet. To enhance the utility and accuracy of the information gathered in each conversation, we match the incomplete or inaccurate names with actual code elements in the buggy programs using our postprocessing process (see Section 3.2.3). Specifically, when getting a function call from LLMs, we check if the code element specified by the given argument of the call exists in the buggy program. If there is no code element named with the given argument, we call the postprocessing process shown in Algorithm 1 with the argument and the fully qualified names of all counterparts in the buggy program. For instance, we get the FQNs of all methods in the program to match with the given argument getOffsetFromLocal, which is provided by the LLM as a method's name for the function

call get\_code\_snippet\_of\_method. These function calls enable LLMs to autonomously get and understand adequate code information in the repository for fault localization.

Previous work [52] finds that only a few files contain buggy methods, which account for a small fraction of the software system. In addition, functions like get\_classes\_of\_path often return plenty of class names that are unrelated to the bug, thus consuming a significant portion of the context length and leaving limited tokens for LLMs to retrieve and inspect code snippets. Considering that the text descriptions of both bug reports and trigger tests usually contain incomplete or fully qualified names of bug-related classes or methods, we design two functions that start with "find", which perform fuzzy searches to localize entities based on incomplete names and assist LLMs in obtaining the full qualified names of suspicious methods rapidly. These function calls are implemented by passing the argument given by LLMs and the FQNs of counterparts to fuzzy search to our postprocessing process (see Section 3.2.3). With these functions for fuzzy search, LLMs can rapidly pinpoint entities mentioned in bug reports and trigger tests, which are likely related to bugs.

Additionally, as mentioned in Section 3.2.1, there is a fixed function call exit(). It allows LLMs to flexibly terminate Step 2 (i.e., Interaction with function calls) early via calling exit() to convey that they are confident in localizing bugs in Step 3 (see Section 3.2.1). This exit mechanism

#### **Algorithm 1** Postprocessing Process

**Input:** The name of query *query*; The names of entities to search *entities*.

**Output:** The matching names *names*.

```
1: names = []
2: query\_split = split(query)
 3: for entity in entities do
 4:
       entity\_splits = split(entity)
 5:
      if query_split all in entity_splits then
 6:
          names.add(entity)
 7: if length(names) > 0 then return names
 8: for entity in entities do
       edit_distance = Levenshtein.distance(query, entity)
      edit_distances.add(edit_distance)
10:
11:
      if edit\_distance < 5 then
12:
          names.add(entity)
13: if length(names) > 0 then return names
14: return names[:5]
```

helps prevent LLMs from the interference of unrelated information extracted in redundant iterations when the number of loops is fixed.

# 3.2.3 Postprocessing process

As mentioned before, we design a postprocessing process to match LLMs' inaccurate output with actual code elements in the buggy program, which helps provide more information in the limited context during the step of interaction with function calls and assists in pinpointing suspicious methods in the step of summarization. The postprocessing process, as detailed in Algorithm 1, has two primary inputs: an inaccurate name provided by LLMs and the fully qualified names of all counterparts in the buggy program. Specifically, the algorithm begins by splitting the query and the entity names using delimiters such as '.', '/', and '('. The algorithm checks if the split components from the entity names contain all segments of the query. If a complete match is found, these names are returned as correct matches. If no exact matches are found, the algorithm proceeds to measure the Levenshtein distance between the query and each entity name. The algorithm prioritizes entity names with a Levenshtein distance of less than five, based on empirical findings that this threshold works well for the types of names typically found in our scenario. If no names meet this threshold, the algorithm returns the five closest matches.

#### 3.2.4 Agent4SR

We designed an agent named Agent4SR to narrow down the search space for FL. Agent4SR aims at global searching bug-related methods in the whole repository. To achieve the goal, besides the basic function calls starting with "get" (e.g., get\_path) for obtaining code information, Agent4SR also uses function calls starting with "find" (e.g., find\_class) for fuzzy searching in huge code space. Following the pipeline in Section 3.2.1, with the given input (i.e., bug reports and trigger tests) and descriptions of all the designing function calls, LLMs are prompted to analyze the bug and search globally for relevant information. For example, for the bug Time-25 presented in Table 1, Agent4SR first

finds class <code>DateTimeZone</code> mentioned in the bug report and then gets its methods. After extracting global information from the whole repository, Agent4SR finally provides top-k suspicious methods for localization refinement.

# 3.2.5 Agent4LR

After obtaining the candidate list from space reduction, FlexFL leverages another agent Agent4LR to perform a local exact search and refine the candidate list. Different from Agent4SR, we only provide Agent4LR with the get\_code\_snippet\_of\_method and exit function calls because we want this agent to save more attention and context length to focus on checking the code snippets of suggested methods in the given candidate list. Through selecting suggested methods to scrutinize their code snippets, Agent4LR finally localizes buggy methods from the candidate list. Since the fully qualified names of the suspicious methods are all given and open-source LLMs have difficulty retelling them, we call the function get\_code\_snippet\_of\_method with the index of the candidate method, helping Agent4LR better focus on double-checking. In addition, we append the fully qualified name of the method that is double-checked via its index in the candidate list to the code snippet retrieved by the function call. This can remind the LLMs of the connection between the code snippet and the fully qualified name of the method for the summarization step.

#### 4 EXPERIMENTAL SETTING

# 4.1 Research Questions

We investigate the following research questions:

- **RQ1:** How does FlexFL compare to other FL techniques? We evaluate the effectiveness of FlexFL by comparing it with leading FL techniques on the Defects4J benchmark.
- RQ2: How effective are the design choices in FlexFL? We compare the performance of FlexFL with its variants on the Defects4J benchmark to illustrate the effectiveness of its components.
- RQ3: Can FlexFL effectively localize bugs based on different open-source LLMs? We investigate the generalizability of our FlexFL by evaluating its performance on different open-source LLMs on the Defects4J benchmark.
- RQ4: Can Agent4SR and FlexFL effectively navigate and localize bugs in the wild? To minimize potential data leakage, we conduct experiments on the GHRB dataset to evaluate the practicality of FlexFL.

#### 4.2 Datasets

Defects4J is a widely used benchmark for automatic fault localization, comprising a manually curated collection of real-world bugs from 17 Java projects [30], [53]. Defects4J (v2.0.0) includes a total of 835 bugs, among which all of the bugs are paired with developer-written trigger tests, and 814 bugs are paired with bug reports.

#### 4.3 Baselines

To investigate the performance of FlexFL, we select state-ofthe-art FL techniques of different families as baselines:

- Information Retrieval-based FL (IRFL): We compare FlexFL with BoostNSift [6] which is the state-of-the-art among method-level IRFL techniques that utilize merely bug reports. However, BoostNSift needs historical bug reports as input, which is not available in our input. To run it in our datasets, we remove the component of BoostNsift that requires historical bug reports, refer to the modified version as BoostN.
- Spectrum-Based FL (SBFL): We consider two most commonly used formula-based SBFL techniques, i.e., Ochiai [7] and Dstar [8], which are also used by prior LLM-based FL studies [25], [26].
- Mutation-based FL (MBFL): We consider two representative MBFL techniques, MUSE [39] and Metallaxis [40] following prior LLM-based FL studies [25].
- LLM-based FL: We compare FlexFL with existing method-level LLM-based FL techniques AutoFL [25] and AgentFL [26].
- **HybridFL**: We compare FlexFL with the state-of-the-art unsupervised technique SBIR [11] that utilizes both bug reports and test cases to our best knowledge. SBIR performs FL at the statement level. To compare FlexFL with it, we transfer the ranked statement list produced by SBIR to the method level as follows. First, we replace each statement in the ranked list with the method it belongs to. If a statement is out of any method, i.e., a field declaration in a class, we remove it from the ranked list. Then, we scan the ranked list from the top and only collect a method when it is scanned for the first time to get the methodlevel rank. SBIR provides 10 results on 815 bugs with different random seeds that are used for the Monte Carlo algorithm [46] to combine its IRFL and SBFL ranks. We choose its FL results when the seed is set to 1 to compare FlexFL with it.

# 4.4 Evaluation Metric

We use three evaluation metrics, i.e., Top-N, MAP, and MRR, which are widely used in the field of fault localization [6], [10], [11], [25], [39]. The higher value of each metric represents better performance.

**Top-N:** Top-N computes the number of bugs with at least one buggy element appearing in the Top-N positions of the recommendation list. The Top-N metric has the additional benefit that it is a closer measure of what developers expect from FL [54]. As suggested by prior work [55], usually, programmers only inspect a few buggy elements at the top of the given ranked list, e.g., 73.58% developers only inspect Top-5 elements [54], we use Top-N (N=1, 3, 5).

MAP: Mean Average Precision (MAP) [56] measures the average position of all the buggy methods localized by the bug localization method in the recommendation list. The definition is as follows:

$$\begin{split} MAP &= \frac{1}{n} \sum_{j=1}^{n} AvgP_j \\ AvgP_j &= \frac{1}{|K_j|} \sum_{k \in K_j} Prec@k \\ Prec@k &= \frac{1}{k} \sum_{i=1}^{k} IsRelevant(i) \end{split}$$

Here,  $AvgP_j$  is the average precision for the j-th bug, and  $|K_j|$  is the total number of buggy methods for the j-th bug. Prec@k represents the precision of the top k methods in the recommendation list, and IsRelevant(i) returns 1 if the i-th method in the recommendation list is responsible for the bug, and 0 otherwise.  $K_j$  are ranks of buggy methods of the j-th bug.

MRR: Mean Reciprocal Rank (MRR) [57] measures the position of the first buggy method localized by the bug localization method in the recommendation list. The definition is as follows:

$$MRR = \frac{1}{n} \sum_{j=1}^{n} \frac{1}{rank_j}$$

Here,  $rank_j$  represents the ranking position of the first buggy method modified to fix the j-th bug in the recommendation list.

#### 4.5 Implementation Details

We build FlexFL mainly based on the LLM Meta-Llama-3-8B-Instruct [16], which is one of the state-of-the-art open-source LLMs and lightweight enough to conduct abundant experiments cheaply, rapidly, and greenly. In order to make our experiments easy to reproduce, we set the temperature to 0.0 and top\_p to 1.0. In this work, we set the initial value of MAX to 10 and the value of k to 5 for our pipeline of agents (see Figure 2) following prior work [25]. We set the value of m, i.e., the size of the candidate list produced in the space reduction stage, to 20, due to the limited context length of LLMs.

In the space reduction stage, FlexFL combines Agent4SR with non-LLM-based FL techniques. In our implementation of FlexFL, we consider the non-LLM-based FL techniques as follows. For IRFL approaches, we choose the SOTA methodlevel IRFL technique BoostN [6]. For SBFL approaches, we select Ochiai [7], which is proven to be one of the most effective ranking strategies in object-oriented programs [2] and is widely used by most FL tools that take test suites as input [11], [39], [58]. Following prior work [11], we use GZoltar(v1.7.2) [59] to reproduce the FL results of Ochiai. MBFL techniques need to modify all possible statements in the program and execute test cases multiple times, thus consuming hours to localize bugs [2], [25]. Therefore, we do not use MBFL techniques [39], [40] for space reduction. When bug reports and test cases are both available, we use the SOTA unsupervised HybridFL technique SBIR [11] in the space reduction stage. SBIR has been evaluated on the Defects4J dataset by Manish et al. [11], thus we directly utilize their evaluation results for experiments. As mentioned, SBIR provides 10 results and we choose its FL results when the seed is set to 1 to ensure the reproducibility of our approach. In this work, we also do not consider learning-based fault localization techniques since they need additional datasets for training, which are not available in unsupervised scenarios.

To combine Agent4SR with non-LLM-based FL techniques and obtain m=20 suspicious methods, FlexFL gets the top-5 ranks of SBIR, Ochiai, BoostN, and Agent4SR successively in the localization refinement stage when bug reports and trigger tests are both available. If only trigger

TABLE 3
FlexFL vs other FL techniques on Defects4J (v2.0.0)

Family	Technique	Top-1	Top-3	Top-5	MAP	MRR
IRFL	BoostN	149	241	280	0.206	0.235
SBFL	Ochiai	167	316	389	0.259	0.297
HybridFL	SBIR	222	377	433	0.309	0.362
LLM-based	FlexFL	350	478	529	0.439	0.501

tests are available, FlexFL gets the top 15 suggested methods of Ochiai and the top 5 of Agent4SR. Similarly, FlexFL gets the top 15 suggested methods of BoostN and the top 5 of Agent4SR when only bug reports are available.

#### 5 EVALUATION

In this section, we present our experimental results in detail with respect to the research questions introduced in Section 4.1.

#### 5.1 RQ1. Overall Performance of FlexFL

We evaluate the overall performance of our FlexFL with quantitative analysis by comparing it with existing FL techniques on the Defects4J dataset and illustrate in detail why FlexFL works through a case study.

# 5.1.1 Quantitative Analysis:

Our FlexFL is compared with existing FL techniques, both non-LLMs-based FL and LLM-based FL techniques, to demonstrate its excellent capability of bug localization.

Table 3 presents a performance comparison between our FlexFL and baselines (i.e., BoostN, Ochiai, and SBIR) in localizing buggy methods on the Defects4J (v2.0.0) dataset. Evaluation results show that our FlexFL successfully localizes 350 bugs within Top-1, 478 bugs within Top-3, and 529 bugs within Top-5, significantly surpassing all baseline techniques on the Defects4J (v2.0.0) benchmark. This highlights the effectiveness of FlexFL in fault localization. Also, the MRR and MAP values of FlexFL are the best among all studied techniques, which demonstrate the high performance of FlexFL in localizing multiple methods.

When compared with LLM-based techniques, it is expensive to reproduce the results of AutoFL on all 835 bugs in Defects4J (v2.0.0), which requires API calling for GPT-3.5 and GPT-4. Therefore, we compare FlexFL to the performance of AutoFL reported in its paper [25]. Note that AutoFL's evaluation is limited to 353 active bugs in five projects of Defects4J (v1.0) (i.e., Chart, Closure, Lang, Math, Time), which is a subset of Defects4J (v2.0.0). Additionally, AutoFL does not use MAP and MRR as evaluation metrics. To ensure a fair comparison, we also evaluate FlexFL on the dataset used by AutoFL in the Top-N metrics. Table 4 shows the comparative results of FlexFL against AgentFL and other baselines (i.e., Muse, Metallaxis, Ochiai, DStar, and AutoFL) on all active bugs in Defects4I (v1.0) following AutoFL [25]. Compared to MBFL and SBFL baselines, FlexFL consistently localizes more bugs across all settings, including Top-1, Top-3, and Top-5. Built on the open-source LLM Llama3-8B, which not only ensures greater transparency of our approach but also enhances data security, FlexFL outperforms

TABLE 4
FlexFL vs vs other FL techniques on Defects4J (v1.0)

Family	Technique	Top-1	Top-3	Top-5
MBFL	MUSE	73	139	161
	Metallaxis	106	162	191
SBFL	Ochiai	122	192	218
	DStar	125	195	216
LLM-based	AgentFL	144	169	173
	AutoFL-GPT-3.5	146	180	194
	FlexFL	<b>164</b>	<b>214</b>	<b>236</b>
	AutoFL-GPT-4	187	236	251

LLM-based FL approaches AgentFL and AutoFL, both of which use GPT-3.5. This superior performance highlights the effectiveness of FlexFL in accurately identifying more bug locations with open-source LLMs. AutoFL with GPT-4 achieves the best performance among all the methods. However, the performance of FlexFL in terms of Top-3 and Top5 is close to AutoFL-GPT-4. It is also worth mentioning that GPT-4 is an expensive closed-source model, while the underlying model of FlexFL is Llama3-8B, which is relatively smaller, cheaper to use, and can be self-hosted to address the concerns about data privacy. Therefore, we believe FlexFL provides unique benefits compared to existing LLM-based FL techniques.

#### 5.1.2 Overlap of Different Methods:

We analyze the overlap of bugs localized in Top-1 between FlexFL and other FL techniques on Defects4J (v2.0.0). As shown in Figure 3, FlexFL successfully localizes 93 bugs that other methods miss at Top-1. This demonstrates that FlexFL can complement and enhance existing non-LLM-based FL approaches, rather than just combining with them.

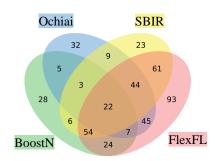


Fig. 3. Overlap Analysis of FlexFL and other FL techniques

#### 5.1.3 Case study

To further investigate the performance of our FlexFL and illustrate why it can work, we conduct a case study using the bug detailed in Table 1. The buggy method is ranked 9th, 53th, and 9th by BoostN, Ochiai, and SBIR, respectively. However, our FlexFL can rank it within the top 1. The following details illustrate how FlexFL effectively localizes the buggy method.

In the first stage of FlexFL, based on the bug report, Agent4SR reasons that this bug is related to DateTimeZone.getOffsetFromLocal method, which is responsible for calculating the offset from local time to UTC., as shown

# TABLE 5 Case Study of Example Bug: Time-25 in Defects4J

Buggy method	org.joda.time.DateTimeZone.getOffsetFromLocal(long)
Agent4SR	Reason: Based on the bug report and the trigger test, I can identify the following:  1. The bug is related to the DateTimeZone.getOffsetFromLocal method, which is responsible for calculating the offset from local time to UTC.  2. The bug is triggered during a DST (Daylight Saving Time) transition, where the offset changes from -7 to -8.  3. The trigger test is related to the Moscow timezone, which also has a DST transition.  Function Calls: 1. find_class("DateTimeZone") 2. get_methods_of_class("org.joda.time.DateTimeZone") 3. get_code_snippet_of_method("getOffsetFromLocal")  Top_1: org.joda.time.tz.FixedDateTimeZone.getOffsetFromLocal(long)  Top_3: org.joda.time.tz.DefaultNameProvider.getOffsetFromLocal(long)
Agent4LR	Reason: Based on the bug report and the trigger test, I can identify the following key points:  1. The bug is related to the DateTimeZone.getOffsetFromLocal method, specifically during DST transitions.  2. The test case provided shows that the method is returning the wrong offset for a specific date and time.  3. The trigger test is failing, indicating that the method is not handling the DST transition correctly.  Function Calls: 1.get_code_snippet_of_method(1) (i.e., org.joda.time.DateTime.DateTime(long,DateTimeZone))  2.get_code_snippet_of_method(18) (i.e., org.joda.time.DateTimeZone.getOffsetFromLocal(long))  Top_1: org.joda.time.DateTimeZone.getOffsetFromLocal(long)

in Table 5. According to this clue, Agent4SR finds the class DateTimeZone and gets the code snippet of method getOffsetFromLocal with the assistance of function calls. Then our function call returns the FQN of the class DateTimeZone, i.e., org.joda.time.DateTimeZone, and the methods named getOffsetFromLocal, which are in the org.joda.time.DateTimeZone class and the org.joda.time.tz.FixedDateTimeZone class. However, due to the limited performance of the used open-source LLM, Agent4SR is confused by the word Fixed in the second method name and thus localizes this wrong method at the top 1. In addition, Agent4SR provides a method that does not exist in the buggy program in the third place, probably due to the hallucination [29] of the open-source LLM. In the summarization stage of Agent4SR, our postprocessing process is used to further match each predicted name with the FQNs of all the methods in the buggy program. The FQN of the buggy method, i.e., org.joda.time.DateTimeZone.getOffsetFromLocal (long), has the minimum editing distance from the third predicted name. Thus, Agent4SR localizes the buggy method in the third place.

In the second stage of FlexFL, Agent4LR automatically checks the suspicious methods localized by SBIR, Ochiai, BoostN, and Agent4SR, which are arranged in order, to localize the buggy method. Although the buggy method is ranked 18th in the candidate list produced by the first stage, as shown in Table 5, Agent4LR succeeds in locating it at top-1, demonstrating the benefits of Agent4LR.

In conclusion, different FL techniques used in the space reduction stage, including LLM-based Agent4SR and non-LLM-based approaches, complement each other and suggest methods comprehensively via extracting information from bug reports and trigger tests in various ways. In the localization refinement stage, Agent4LR can refine the result of the first stage and perform more accurate localization. In addition, the function calls and the postprocessing process contribute to assisting agents in efficiently obtaining information relevant to bugs from the huge code base of the whole repository.

TABLE 6 Ablation study on input

Variant	Top-1	Top-3	Top-5	MAP	MRR
w/o trigger test w/o bug report w/o buggy program	257 266 45	345 395 64	387 442 75	0.323 0.339 0.062	0.365 0.399 0.066
FlexFL	350	478	529	0.439	0.501

Answer to RQ1: Our FlexFL outperforms existing fault localization techniques on Defects4J v1.0 and v2.0.0. Moreover, it can localize 93 unique bugs that cannot be localized by the non-LLM-based FL techniques used in the space reduction stage.

# 5.2 RQ2. Ablation Study

We conduct comprehensive ablation studies to investigate the impacts of different inputs and design choices on the effectiveness of FlexFL.

# 5.2.1 Ablation of Inputs

We first compare the roles of different inputs in FlexFL. From Table 6, we can observe that FlexFL, which takes both bug reports and test cases as input, significantly outperforms FlexFL w/o trigger test and FlexFL w/o bug reports. By flexibly leveraging available bug-related information, FlexFL can localize at least 31.6% more bugs at top-1, which indicates the effectiveness of flexibility in handling inputs that the existing LLM-based FL techniques lack.

We also evaluate the performance of the basic variant of FlexFL that is not provided with function calls to access any information in the buggy program and directly localizes bugs with bug reports and test cases. Table 6 shows that FlexFL without buggy program can only localize 75 bugs at top-5 even with suspicious methods localized by the state-of-the-art non-LLM-based FL techniques, demonstrating that the tool use greatly improves the performance of FlexFL and the impact of model memorization is limited.

TABLE 7
Ablation study on two-stage

Variant	Top-1	Top-3	Top-5	MAP	MRR
BoostN	149	241	280	0.206	0.235
BoostN + Agent4LR	255	336	364	0.317	0.356
Ochiai	167	316	389	0.259	0.297
Ochiai + Agent4LR	303	421	475	0.387	0.442
SBIR	222	377	433	0.309	0.362
SBIR + Agent4LR	319	429	473	0.400	0.453
FlexFL w/o Agent4SR	338	467	510	0.422	0.485
FlexFL	350	<b>478</b>	<b>529</b>	<b>0.439</b>	<b>0.501</b>

# 5.2.2 Ablation of Design Choices

We investigate the contributions of the two-stage design and different design choices for assisting agents to better interact with function calls.

**Two-stage Design:** FlexFL is composed of two stages, i.e., space reduction and localization refinement, and we design two agents for each stage, i.e., Agent4SR and Agent4LR. The localization refinement stage requires the candidate list produced by the space reduction stage. Therefore, we cannot entirely remove the space reduction stage and thus focus on the effectiveness of combining different FL techniques in this stage. We construct multiple variants of FlexFL, each of which only uses one FL technique to produce top-20 suspicious methods in the first stage, and compare them with FlexFL. To investigate the effectiveness of the localization refinement stage, we compare these variants with the FL technique they use. In addition, to investigate the contribution of Agent4SR, we construct a variant by removing Agent4SR from the first stage, i.e., FlexFL without Agent4SR, and compare it with FlexFL.

Table 7 shows the evaluation results. First, FlexFL can achieve the best performance compared to all these variants, suggesting the effectiveness of the space reduction stage. Second, the variants that leverage Agent4LR, e.g., SBIR + Agent4LR, outperform their used non-LLM-based FL techniques, e.g., SBIR, indicating that Agent4LR, as well as the localization refinement stage, can improve non-LLM-based FL techniques of various families. For instance, Agent4LR refines the results of Ochiai and increases its top-1 score by 81.4%. Third, FlexFL outperforms FlexFL without Agent4SR, demonstrating that the synergy between Agent4SR and non-LLM-based FL techniques can complement each other's advantages and enhance bug localization. To conclude, our two-stage design combines and refines the results of LLM-based and non-LLM-based FL approaches, which helps FlexFL improve existing FL techniques.

Designs for better interaction with function calls: To release the power of open-source LLMs, FlexFL designs three components to assist them in better interaction with function calls to extract information from the buggy program effectively. First, FlexFL prompts open-source LLMs to reason and plan how to use function calls before interacting with them. Second, FlexFL designs a postprocessing process to match inaccurate names provided by open-source LLMs to actual code elements in the repository. Third, Agent4LR adapts the parameter of get\_code\_snippet\_of\_method to the method's number in the candidate list and append the

TABLE 8
Ablation study on designs for better tool use

Variant	Top-1	Top-3	Top-5   MA	P MRR
w/o reasoning w/o postprocessing w/o focus	330 330 332	466 462 440	512   0.41 512   0.41 479   0.40	7 0.478
FlexFL	350	478	529   0.43	39 0.501

TABLE 9
Comparison of FlexFL based on different open-source LLMs on Defects4J (v2.0.0)

Base Model	Top-1	Top-3	Top-5	MAP	MRR
Mistral-Nemo-12B	322	464	507	0.411	0.473
Qwen2-7B	329	456	500	0.408	0.474
Llama3-8B	350	<b>478</b>	<b>529</b>	<b>0.439</b>	<b>0.501</b>

FQN of the method checked to its code snippet. To prove the usefulness of these three designs, we evaluate one variant of FlexFL that interacts with function calls directly without reasoning, one variant that does not use the postprocessing process, and another that uses the same parameter as Agent4SR to use <code>get\_code\_snippet\_of\_method</code> in the second stage, namely w/o focus.

Results are shown in table 8. Compared to these variants, FlexFL can localize at most 50 more bugs at top-5 and improve up to 8% on both MAP and MRR metrics, indicating the effectiveness of our designs for assisting open-source LLMs in better interaction with function calls.

**Answer to RQ2:** All design choices of FlexFL make contributions to the whole framework's performance, the most significant of which is the flexibility of making use of different types of input, which improves FlexFL at least 31.6% on the top-1 metric.

#### 5.3 RQ3. Generalizability of FlexFL

To investigate the generalizability of FlexFL across different open-source LLMs, we also implement FlexFL based on two other lightweight open-source LLMs, i.e., Qwen2-7B-Instruct [17] and Mistral-Nemo-12B-Instruct [31], respectively, and evaluate the two variants on Defects4J (v2.0.0). Qwen2-7B and Mistral-Nemo-12B are famous lightweight open-source models and achieve state-of-the-art performances across various tasks [60]. Table 9 presents the evaluation results. The variants of FlexFL based on different LLMs achieve slightly different performances, indicating that the base model has an impact on the effectiveness of FlexFL. Among these variants, FlexFL-Llama3-8B achieves the best performance in all metrics. Additionally, the performance of FlexFL-Qwen2-7B and FlexFL-Mistral-Nemo-12B is comparable to FlexFL-Llama3-8B, which indicates that FlexFL can generally work with different lightweight opensource LLMs.

**Answer to RQ3:** FlexFL demonstrates good generalizability in working with different lightweight open-source LLMs.

# 5.4 RQ4. Practicality of FlexFL

Considering the LLM used in FlexFL (see section 4.5) was trained with data collected until March 2023 [61], the Defects4I dataset is not free from data leakage concerns. To mitigate such concerns, we also conduct experiments on the GHRB dataset [32], which was recently collected from 17 GitHub repositories that use JUnit. We evaluate both FlexFL and Agent4SR on a subset GHRB where the bugs are fixed after the training data cutoff point (i.e., March 2023) of Llama3. This subset contains 38 bugs. Table 10 shows the quantitative complexity of the GHRB subset and Defects4J (v2.0.0), including the average number of files and code lines contained in the buggy program and the faulty methods needed to be edited to fix the corresponding bugs. The bugs in this dataset are notably more complex than those found in Defects4J, allowing for a more rigorous evaluation of our approach. Due to the immaturity of the GHRB dataset, i.e., the scripts provided in it often cannot successfully compile the buggy program, and the difficulty of dynamically executing a complex program to collect coverage information, we failed to reproduce the baselines that need dynamic runtime information, i.e., Ochiai, SBIR, AgentFL, and AutoFL. Therefore, we only evaluate a variant of FlexFL that utilizes only bug reports and compare it to BoostN.

TABLE 10 Complexity of GHRB and Defects4J (v2.0.0)

Dataset	Files	Faulty Methods	LoC*
Defects4J (v2.0.0)	267	1.73	76.3k
GHRB	895	2.5	157.3k

<sup>\*</sup> LoC is the average number of code lines for each buggy program.

Table 11 shows the evaluation results of FlexFL against BoostN, Agent4SR on the GHRB subset. The results demonstrate that both Agent4SR and FlexFL outperform BoostN in terms of Top-1, Top-3, and Top-5. Moreover, FlexFL achieves the best performance, confirming the effectiveness of the synergy between Agent4SR and BoostN. In addition, FlexFL localizes 12 out of 38 bugs (i.e., 31.6%) in the GHRB dataset at top-1 with only bug reports, which is close to its corresponding evaluation results on the Defects4J dataset, i.e., locating 257 of 814 bugs (i.e., 31.5%), shown in table 6. These experiment results demonstrate the practicality of FlexFL and indicate that the impact of data leakage is limited.

TABLE 11
Comparison of FlexFL with Baselines on GHRB

Technique	Top-1	Top-3	Top-5	MAP	MRR
BoostN	4	8	11	0.104	0.168
Agent4SR	11	13	13	0.280	0.311
FlexFL	<b>12</b>	<b>15</b>	<b>15</b>	<b>0.280</b>	<b>0.355</b>

**Answer to RQ4:** Evaluation results on the GHRB dataset demonstrate the good practicality of both FlexFL and Agent4SR, indicating that the impact of data leakage is limited.

# **6 THREATS TO VALIDITY**

Internal Validity concerns the possibility of data leakage and selection bias in the experiment. While Defects4J has been commonly used in prior research, the fixes of its collected bugs may have been seen by the used LLM during pre-training, leading to the risk of data leakage. However, as shown in Section 5.2.1, FlexFL performs poorly without buggy programs as input. Also, the evaluation results of FlexFL on the GHRB dataset are comparable to those on the Defects4J dataset (c.f. Section 5.4. These results can support that the effectiveness of FlexFL is not simply due to the memorization of the used LLM. Thus, we believe the threat of data leakage is limited.

External Validity concerns whether the results presented would generalize. We only evaluate our approach on Java projects. It is difficult to tell whether the evaluation results would generalize to projects in other languages. However, Java is one of the most popular languages and Defects4J is widely used by prior fault localization studies. In addition, our method is dataset-independent and language-agnostic. We plan to apply our approach to other datasets, real-world scenarios, and other programming languages in the future.

# 7 CONCLUSION AND FUTURE WORK

We propose FlexFL, a flexible and effective LLM-based FL technique that can work with lightweight open-source LLMs. FlexFL improves FL techniques in general scenarios utilizing a two-stage process: (1) narrowing down the search space of buggy code using state-of-the-art FL techniques of different families and (2) leveraging LLMs to delve deeper into understanding the root causes of bugs via doublechecking the code snippets of the methods selected by the first stage. To enable LLMs to leverage flexible types of bugrelated information, FlexFL designs prompt templates and LLM-based agents without assuming the existence of any specific type of bug-related information. To make FlexFL work with lightweight open-source LLMs, which suffer more from long input and usually have no out-of-the-box function call capabilities, we design a general manner of interaction with function calls that enable the construction of agents based on any chat model. Evaluation results show that FlexFL with a lightweight open-source LLM Llama3-8B can locate 42 and 63 more bugs than two state-of-the-art LLM-based FL approaches AutoFL and AgentFL that both use GPT-3.5. FlexFL also demonstrates good generalization in working with different open-source LLMs and great practicality in locating bugs in the wild. In the future, we plan to apply our approach to other datasets, real-world scenarios, and other programming languages.

#### REFERENCES

- [1] W. E. Wong, R. Gao, Y. Li, R. Abreu, and F. Wotawa, "A survey on software fault localization," *IEEE Transactions on Software Engineering*, vol. 42, no. 8, pp. 707–740, 2016.
- [2] D. Zou, J. Liang, Y. Xiong, M. D. Ernst, and L. Zhang, "An empirical study of fault localization families and their combinations," IEEE Transactions on Software Engineering, vol. 47, no. 2, pp. 332–347, 2021.
- [3] K. C. Youm, J. Ahn, J. Kim, and E. Lee, "Bug localization based on code change histories and bug reports," in 2015 Asia-Pacific Software Engineering Conference (APSEC), 2015, pp. 190–197.

- [4] S. Tsumita, S. Hayashi, and S. Amasaki, "Large-scale evaluation of method-level bug localization with finerbench4bl," in 2023 IEEE International Conference on Software Analysis, Evolution and Reengineering (SANER), 2023, pp. 815–824.
- [5] W. Zhang, Z. Li, Q. Wang, and J. Li, "Finelocator: A novel approach to method-level fine-grained bug localization by query expansion," INFORMATION AND SOFTWARE TECHNOLOGY, vol. 110, pp. 121–135, JUN 2019.
- [6] A. Razzaq, J. Buckley, J. V. Patten, M. Chochlov, and A. R. Sai, "BoostNSift: A query boosting and code sifting technique for method level bug localization," in 2021 IEEE 21st International Working Conference on Source Code Analysis and Manipulation (SCAM). IEEE, 2021, pp. 81–91.
- [7] R. Abreu, P. Zoeteweij, and A. J. van Gemund, "On the accuracy of spectrum-based fault localization," in Testing: Academic and Industrial Conference Practice and Research Techniques - MUTATION (TAICPART-MUTATION 2007), 2007, pp. 89–98.
- [8] W. E. Wong, V. Debroy, R. Gao, and Y. Li, "The dstar method for effective software fault localization," *IEEE Trans. Reliab.*, vol. 63, no. 1, pp. 290–308, 2014.
- [9] M. Zhang, Y. Li, X. Li, L. Chen, Y. Zhang, L. Zhang, and S. Khurshid, "An empirical study of boosting spectrum-based fault localization via pagerank," *IEEE Transactions on Software Engineering*, vol. 47, no. 6, pp. 1089–1113, 2021.
- [10] X. L. Yiling Lou, Ali Ghanbari and et al., "Can automated program repair refine fault localization? a unified debugging approach," in ISSTA '20: 29th ACM SIGSOFT International Symposium on Software Testing and Analysis, Virtual Event, USA, July 18-22, 2020, S. Khurshid and C. S. Pasareanu, Eds. ACM, 2020, pp. 75–87.
- [11] M. Motwani and Y. Brun, "Better automatic program repair by using bug reports and tests together," in 2023 IEEE/ACM 45th International Conference on Software Engineering (ICSE), 2023, pp. 1225–1237.
- [12] T. B. Le, R. J. Oentaryo, and D. Lo, "Information retrieval and spectrum based bug localization: better together," in *Proceedings of* the 2015 10th Joint Meeting on Foundations of Software Engineering, ESEC/FSE 2015, Bergamo, Italy, August 30 - September 4, 2015, E. D. Nitto, M. Harman, and P. Heymans, Eds. ACM, 2015, pp. 579–590.
- [13] H. J. Mark Chen, Jerry Tworek and et al., "Evaluating large language models trained on code," CoRR, vol. abs/2107.03374, 2021.
- [14] OpenAI, "GPT-4 technical report," CoRR, vol. abs/2303.08774, 2023
- [15] F. G. Baptiste Rozière, Jonas Gehring and et al., "Code llama: Open foundation models for code," CoRR, vol. abs/2308.12950, 2023.
- [16] "Blog of Meta Llama 3." https://ai.meta.com/blog/meta-llama-3/, 2024.
- [17] "Blog of Qwen2." https://qwenlm.github.io/blog/qwen2/, 2024.
- [18] D. Y. Daya Guo, Qihao Zhu and et al., "Deepseek-coder: When the large language model meets programming - the rise of code intelligence," CoRR, vol. abs/2401.14196, 2024.
- [19] S. Yao, J. Zhao, D. Yu, N. Du, I. Shafran, K. R. Narasimhan, and Y. Cao, "React: Synergizing reasoning and acting in language models," in *The Eleventh International Conference on Learning Representa*tions, ICLR 2023, Kigali, Rwanda, May 1-5, 2023. OpenReview.net, 2023.
- [20] V. N. Changan Niu, Chuanyi Li and et al., "An empirical comparison of pre-trained models of source code," in 45th IEEE/ACM International Conference on Software Engineering, ICSE 2023, Melbourne, Australia, May 14-20, 2023. IEEE, 2023, pp. 2136–2148.
- [21] Z. Zeng, H. Tan, H. Zhang, J. Li, Y. Zhang, and L. Zhang, "An extensive study on pre-trained models for program understanding and generation," in ISSTA '22: 31st ACM SIGSOFT International Symposium on Software Testing and Analysis, Virtual Event, South Korea, July 18 22, 2022, S. Ryu and Y. Smaragdakis, Eds. ACM, 2022, pp. 39–51.
- [22] C. S. Xia and L. Zhang, "Conversational automated program repair," CoRR, vol. abs/2301.13246, 2023.
- [23] S. Kang, J. Yoon, and S. Yoo, "Large language models are few-shot testers: Exploring llm-based general bug reproduction," in 45th IEEE/ACM International Conference on Software Engineering, ICSE 2023, Melbourne, Australia, May 14-20, 2023. IEEE, 2023, pp. 2312– 2323.
- [24] Y. Wu, Z. Li, J. M. Zhang, M. Papadakis, M. Harman, and Y. Liu, "Large language models in fault localisation," CoRR, vol. abs/2308.15276, 2023.

- [25] S. Kang, G. An, and S. Yoo, "A quantitative and qualitative evaluation of llm-based explainable fault localization," *Proc. ACM Softw. Eng.*, vol. 1, no. FSE, jul 2024.
- [26] Y. Qin, S. Wang, Y. Lou, J. Dong, K. Wang, X. Li, and X. Mao, "Agentfl: Scaling llm-based fault localization to project-level context," CoRR, vol. abs/2403.16362, 2024.
- [27] R. Widyasari, J. W. Ang, T. G. Nguyen, N. Sharma, and D. Lo, "Demystifying faulty code: Step-by-step reasoning for explainable fault localization," in *IEEE International Conference on Software* Analysis, Evolution and Reengineering, SANER 2024, Rovaniemi, Finland, March 12-15, 2024. IEEE, 2024, pp. 568–579.
- [28] N. F. Liu, K. Lin, J. Hewitt, A. Paranjape, M. Bevilacqua, F. Petroni, and P. Liang, "Lost in the middle: How language models use long contexts," *Transactions of the Association for Computational Linguistics*, vol. 12, pp. 157–173, 2024.
- [29] Y. Zhang, Y. Li, L. Cui, D. Cai, L. Liu, T. Fu, X. Huang, E. Zhao, Y. Zhang, Y. Chen et al., "Siren's song in the ai ocean: a survey on hallucination in large language models," arXiv preprint arXiv:2309.01219, 2023.
- [30] R. Just, D. Jalali, and M. D. Ernst, "Defects4j: a database of existing faults to enable controlled testing studies for java programs," in Proceedings of the 2014 International Symposium on Software Testing and Analysis, ser. ISSTA 2014. New York, NY, USA: Association for Computing Machinery, 2014, p. 437–440.
- [31] "Blog of Mistral-Nemo." https://mistral.ai/news/mistral-nemo/, 2024.
- [32] J. Y. Lee, S. Kang, J. Yoon, and S. Yoo, "The github recent bugs dataset for evaluating llm-based debugging applications," CoRR, vol. abs/2310.13229, 2023.
- [33] "Our replication package." https://doi.org/10.5281/zenodo. 11524997, 2024.
- [34] J. Zhou, H. Zhang, and D. Lo, "Where should the bugs be fixed? more accurate information retrieval-based bug localization based on bug reports," in 34th International Conference on Software Engineering, ICSE 2012, June 2-9, 2012, Zurich, Switzerland, M. Glinz, G. C. Murphy, and M. Pezzè, Eds. IEEE Computer Society, 2012, pp. 14–24.
- [35] K. C. Youm, J. Ahn, and E. Lee, "Improved bug localization based on code change histories and bug reports," *Inf. Softw. Technol.*, vol. 82, pp. 177–192, 2017.
- [36] J. A. Jones and M. J. Harrold, "Empirical evaluation of the tarantula automatic fault-localization technique," in *Proceedings of the 20th IEEE/ACM International Conference on Automated Software Engineering*, ser. ASE '05. New York, NY, USA: Association for Computing Machinery, 2005, p. 273–282.
- [37] Y. Jia and M. Harman, "An analysis and survey of the development of mutation testing," *IEEE Trans. Software Eng.*, vol. 37, no. 5, pp. 649–678, 2011.
- [38] R. DeMillo, R. Lipton, and F. Sayward, "Hints on test data selection: Help for the practicing programmer," *Computer*, vol. 11, no. 4, pp. 34–41, 1978.
- [39] S. Moon, Y. Kim, M. Kim, and S. Yoo, "Ask the mutants: Mutating faulty programs for fault localization," in 2014 IEEE Seventh International Conference on Software Testing, Verification and Validation, 2014, pp. 153–162.
- [40] M. Papadakis and Y. L. Traon, "Metallaxis-fl: mutation-based fault localization," Softw. Test. Verification Reliab., vol. 25, no. 5-7, pp. 605–628, 2015.
- [41] H. Wang, K. Yang, X. Zhao, Y. Cui, and W. Wang, "Contribution-based test case reduction strategy for mutation-based fault localization (s)." in SEKE, 2023, pp. 142–145.
- [42] X. Li, W. Li, Y. Zhang, and L. Zhang, "Deepfl: integrating multiple fault diagnosis dimensions for deep fault localization," in Proceedings of the 28th ACM SIGSOFT International Symposium on Software Testing and Analysis, ISSTA 2019, Beijing, China, July 15-19, 2019, D. Zhang and A. Møller, Eds. ACM, 2019, pp. 169–180.
  [43] J. Sohn and S. Yoo, "FLUCCS: using code and change metrics"
- [43] J. Sohn and S. Yoo, "FLUCCS: using code and change metrics to improve fault localization," in *Proceedings of the 26th ACM SIGSOFT International Symposium on Software Testing and Analysis, Santa Barbara, CA, USA, July 10 - 14, 2017*, T. Bultan and K. Sen, Eds. ACM, 2017, pp. 273–283.
- [44] E. R. Christopher J. C. Burges, Tal Shaked and et al., "Learning to rank using gradient descent," in Machine Learning, Proceedings of the Twenty-Second International Conference (ICML 2005), Bonn, Germany, August 7-11, 2005, ser. ACM International Conference Proceeding Series, L. D. Raedt and S. Wrobel, Eds., vol. 119. ACM, 2005, pp. 89–96.

- [45] T. Kuo, C. Lee, and C. Lin, "Large-scale kernel ranksvm," in Proceedings of the 2014 SIAM International Conference on Data Mining, Philadelphia, Pennsylvania, USA, April 24-26, 2014, M. J. Zaki, Z. Obradovic, P. Tan, A. Banerjee, C. Kamath, and S. Parthasarathy, Eds. SIAM, 2014, pp. 812–820.
- [46] L. Deng, "The cross-entropy method: A unified approach to combinatorial optimization, monte-carlo simulation, and machine learning," *Technometrics*, vol. 48, no. 1, pp. 147–148, 2006.
- [47] P. Vaithilingam, T. Zhang, and E. L. Glassman, "Expectation vs. experience: Evaluating the usability of code generation tools powered by large language models," in *Chi conference on human factors in computing systems extended abstracts*, 2022, pp. 1–7.
  [48] J. Wang, Y. Huang, C. Chen, Z. Liu, S. Wang, and Q. Wang,
- [48] J. Wang, Y. Huang, C. Chen, Z. Liu, S. Wang, and Q. Wang, "Software testing with large language models: Survey, landscape, and vision," *IEEE Transactions on Software Engineering*, 2024.
- [49] J. Zhang, J. Cambronero, S. Gulwani, V. Le, R. Piskac, G. Soares, and G. Verbruggen, "Repairing bugs in python assignments using large language models," arXiv preprint arXiv:2209.14876, 2022.
- [50] "Bug report of Time-25(Defects4J)." https://sourceforge.net/p/joda-time/bugs/90/, 2010.
- [51] F. Liu, Y. Liu, L. Shi, H. Huang, R. Wang, Z. Yang, and L. Zhang, "Exploring and evaluating hallucinations in llm-powered code generation," arXiv preprint arXiv:2404.00971, 2024.
- [52] A. Koyuncu, K. Liu, T. F. Bissyandé, D. Kim, M. Monperrus, J. Klein, and Y. Le Traon, "Ifixr: Bug report driven program repair," in Proceedings of the 2019 27th ACM Joint Meeting on European Software Engineering Conference and Symposium on the Foundations of Software Engineering, ser. ESEC/FSE 2019. New York, NY, USA: Association for Computing Machinery, 2019, p. 314–325.
- Association for Computing Machinery, 2019, p. 314–325.
  [53] M. N. Rafi, A. R. Chen, T.-H. Chen, and S. Wang, "Exploring data cleanness in defects4j and its influence on fault localization efficiency," in *Proceedings of the 2024 IEEE/ACM 46th International*

- Conference on Software Engineering: Companion Proceedings, 2024, pp. 386–387.
- [54] P. S. Kochhar, X. Xia, D. Lo, and S. Li, "Practitioners' expectations on automated fault localization," in *Proceedings of the 25th International Symposium on Software Testing and Analysis*, ser. ISSTA 2016. New York, NY, USA: Association for Computing Machinery, 2016, p. 165–176.
- [55] C. Parnin and A. Orso, "Are automated debugging techniques actually helping programmers?" in *Proceedings of the 2011 Interna*tional Symposium on Software Testing and Analysis, ser. ISSTA '11. New York, NY, USA: Association for Computing Machinery, 2011, p. 199–209.
- [56] C. D. Manning, P. Raghavan, and H. Schütze, Introduction to information retrieval. Cambridge University Press, 2008.
- [57] E. M. Voorhees, "The TREC-8 question answering track report," in Proceedings of The Eighth Text Retrieval Conference, TREC 1999, Gaithersburg, Maryland, USA, November 17-19, 1999, ser. NIST Special Publication, E. M. Voorhees and D. K. Harman, Eds., vol. 500-246. National Institute of Standards and Technology (NIST), 1999.
- [58] M. Zhang, X. Li, L. Zhang, and S. Khurshid, "Boosting spectrum-based fault localization using pagerank," in *Proceedings of the 26th ACM SIGSOFT International Symposium on Software Testing and Analysis, Santa Barbara, CA, USA, July 10 14, 2017*, T. Bultan and K. Sen, Eds. ACM, 2017, pp. 261–272.
- [59] J. Campos, A. Riboira, A. Perez, and R. Abreu, "Gzoltar: an eclipse plug-in for testing and debugging," in 2012 Proceedings of the 27th IEEE/ACM International Conference on Automated Software Engineering, 2012, pp. 378–381.
- [60] "Open LLM Leaderboard of HuggingFace." https://huggingface. co/spaces/open-llm-leaderboard/open\_llm\_leaderboard, 2024.
- [61] "Cutoff date of training dataset of Llama3." https://github.com/meta-llama/llama3/blob/main/MODEL\_CARD.md, 2024.