Modularization is Better: Effective Code Generation with Modular Prompting

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Abstract

Large Language Models are transforming software development by automatically generating code. Current prompting techniques such as Chain-of-Thought (CoT) suggest tasks step by step and the reasoning process follows a linear structure, which hampers the understanding of complex programming problems, particularly those requiring hierarchical solutions. Inspired by the principle of modularization in software development, in this work, we propose a novel prompting technique, called MoT, to enhance the code generation performance of LLMs. At first, MoT exploits modularization principles to decompose complex programming problems into smaller, independent reasoning steps, enabling a more structured and interpretable problem-solving process. This hierarchical structure improves the LLM's ability to comprehend complex programming problems. Then, it structures the reasoning process using an MLR Graph (Multi-Level Reasoning Graph), which hierarchically organizes reasoning steps. This approach enhances modular understanding and ensures better alignment between reasoning steps and the generated code, significantly improving code generation performance. Our experiments on two advanced LLMs (GPT-4o-mini and DeepSeek-R1), comparing MoT to six baseline prompting techniques across six widely used datasets, HumanEval, HumanEval-ET, HumanEval+, MBPP, MBPP-ET, and MBPP+, demonstrate that MoT significantly outperforms existing baselines (e.g., CoT and SCoT), achieving Pass@1 scores ranging from 58.1% to 95.1%. The experimental results confirm that MoT significantly enhances the performance of LLM-based code generation.

Keywords

Code Generation, Prompting Technique, Modularization, Hierarchical Task Decomposition, Intelligent Programming

1 Introduction

Large Language Models (LLMs) are transforming the field of software development [1–4]. In recent years, an increasing number of LLMs have been developed to assist programmers in writing code, such as GPT-4 [5] and DeepSeek [6].

Various prompting techniques have also been introduced to enhance LLM-based code generation, as shown in Figure 1. For example, Chain-of-Thought (CoT) prompting [7] is one of the most widely used prompting techniques, which employs intermediate steps to facilitate step-by-step reasoning in LLMs. CoT has been shown to significantly improve LLMs' problem-solving capabilities without requiring modifications to the model itself. To further enhance the quality of code generation, Li et al. [8] proposed SCoT,

which builds upon CoT prompting by leveraging program structures (i.e., sequence, branch, and loop structures) to generate intermediate reasoning steps. Jiang et al. [9] introduced Self-Planning prompting, which enables LLMs to design a structured step-by-step plan prior to code generation. The LLM creates a comprehensive plan for code generation based on the problem description, which it then executes incrementally. Recently, CodeCoT prompting [10] has integrated CoT with self-examination. The LLM improves the accuracy of generated code by producing initial code and test cases, verifying code execution, and iteratively resolving errors as they are identified. Although existing prompting techniques have been proposed to guide LLMs, they still encounter several limitations due to their monolithic reasoning structure [1, 11]. This rigid structure limits LLMs' capacity to effectively break down complex programming problems into modular and independently solvable subproblems [12].

Analogous to the concept of monolithic programming in traditional software development, prompting techniques such as CoT suggest tasks step by step through a monolithic structure [13, 14]. Before 1970, software development primarily adhered to a linear, monolithic programming paradigm [15]. Although this monolithic approach was relatively effective at the time, its limitations gradually became evident as software size and complexity increased, leading to reduced development efficiency. To address the limitations of the monolithic approach, David Parnas introduced the concept of modularization in software development and highlighted the significance of hierarchical design [15-18]. He noted that by breaking complex problems into smaller, more manageable parts, developers can design and implement systems at a higher level of abstraction. Similarly, while expliciting CoT methods have demonstrated effectiveness in specific tasks, their inherently linear structure limits their capacity to handle complex tasks. Researchers believe that the principles of modularization and hierarchical structure should also be incorporated into the reasoning processes of LLMs [19].

In this paper, we propose the MoT (Modularization of Thoughts) prompting technique for code generation. MoT goes beyond traditional monolithic reasoning by introducing a structured approach that better captures the modular nature of programming problems. At its core, MoT constructs an MLR Graph (Multi-Level Reasoning Graph), where each node represents a code task design, and each edge defines the logical dependencies between tasks. By providing an explicit structure of relationships and functionalities, the MLR Graph enhances LLMs' understanding of modular code components. Inspired by the principle of modularization in software development, MoT decomposes complex programming problems into smaller, independent yet interdependent modules. These modules can be refined, adapted, and recombined, allowing for flexible composition of a coherent final solution. Through this modular

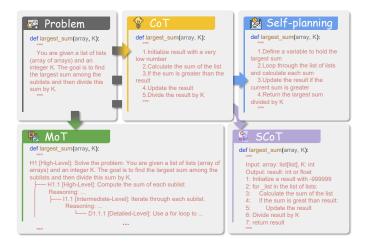


Figure 1: Different Prompting Techniques

and hierarchical approach, MoT enables LLMs to provide better solutions of programming problems.

We conducted extensive experiments to evaluate MoT with two state-of-the-art LLMs (i.e., GPT-4o-mini [5] and DeepSeek-R1 [6]) on six public benchmarks. Our results show that MoT significantly outperforms all the compared prompting techniques with both LLMs on all six benchmarks. For example, MoT achieves an average improvement of 0.03% to 32.85% in Pass@1 across all subjects compared to other techniques. The results show the effectiveness of MoT for improving code generation performance. Moreover, we construct two variants of MoT for the ablation study. The results confirm the contribution of the modularization principles and the MLR Graph prompting strategy to the overall MoT performance. We also conduct an experiment to analyze cost implications, demonstrating that MoT provides an effective approach to code generation.

We summarize our contributions in this work as follows:

- We propose a novel prompting technique, called MoT, to improve the code generation performance of LLMs by incorporating the modularization principles of software development into the reasoning process.
- We design a novel Multi-Level Reasoning Graph to further enhance modular understanding and ensure better alignment between reasoning steps and the generated code.
- We conducted extensive experiments on two LLMs (i.e., GPT-40-mini and DeepSeek-R1) with six benchmarks, comparing them with eight baselines to demonstrate the effectiveness of MoT in improving code generation performance.

2 Background and Related Work

In recent years, LLMs have demonstrated significant potential in the field of code generation [20–25]. Standard language models perform code completion and generation after autoregressive pre-training. Academia and industry have introduced various code LLMs, such as AlphaCode [26], CodeGen [27], CodeGeeX [28], InCoder [29], StarCoder [30], CodeLlama [31], and CodeT5+ [32]. Furthermore, general LLMs, such as ChatGPT [5] and DeepSeek [6], are also widely used for code generation.

Recently, prompting techniques have driven the ongoing advancement of code generation based on LLMs [33]. Zero-shot prompting generates code based solely on the problem description without any examples, while few-shot prompting aids the model in understanding the input-output structure by incorporating examples [34]. To address complex programming problems, various prompting techniques have been proposed, as illustrated in Figure 1. Wei et al. proposed CoT prompting, which requires the model to first generate intermediate reasoning steps to ensure logical coherence [7]. Additionally, researchers introduced Self-planning prompting, which involves formulating a detailed plan prior to coding and executing it incrementally [9]. More recently, Li et al. introduced SCoT prompting, which leverages the sequence, branch, and loop structures of programs to generate reasoning steps, thereby aligning the reasoning process more closely with actual programming logic [8]. Furthermore, CodeCoT prompting combines CoT with a selfexamination mechanism. The model not only generates initial code but also simultaneously generates test cases, verifies code execution, and iteratively repairs errors, thereby continuously improving the accuracy of generated code [10].

However, the existing prompting techniques have several limitations. Most existing prompting techniques rely on monolithic reasoning, in which the model adheres to a sequential reasoning process, failing to explicitly capture the hierarchical and modular nature of programming logic. Although these prompting techniques can improve logical consistency, they remain inadequate for complex programming tasks demanding sophisticated task designs [35–37].

3 Approach

3.1 Overview

We introduce MoT (Modularization-of-Thought Prompting), a novel prompting technique based on MLR graphs (Multi-Level Reasoning), to enhance LLMs' code generation. MoT applies modularization and hierarchical structures to guide logical reasoning and code generation using MLR graphs. Our core idea is to incorporate the modularization principles into the reasoning process. This novel Multi-Level Reasoning graph can improve modular understanding and ensure better alignment between reasoning steps and the generated code.

Figure 2 provides an overview of our method, which comprises two primary phases: (1) the MLR graph generation phase (see Section 3.2 for details), where the model analyzes the problem description, constructs an MLR graph of the programming problem; (2) the code generation phase (see Section 3.3 for details), where the model progressively generates code guided by the hierarchical MLR graph, thereby enhancing code accuracy through the modularization and hierarchical structure.

3.2 MLR Graph Generation Phase

A Multi-Level Reasoning (MLR) graph is a structured representation that systematically structures reasoning steps into prompts, facilitating LLMs' comprehension of complex programming problems. In an MLR graph, each node indicates the rationale for its step by embedding the reasoning process. During the MLR graph

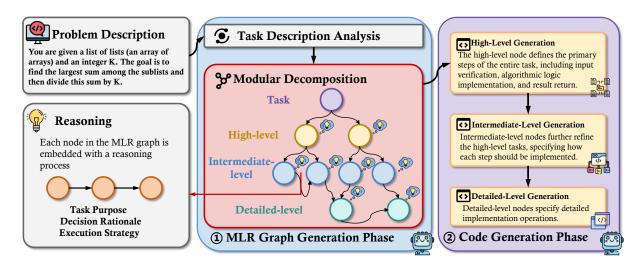


Figure 2: The Overview of MoT

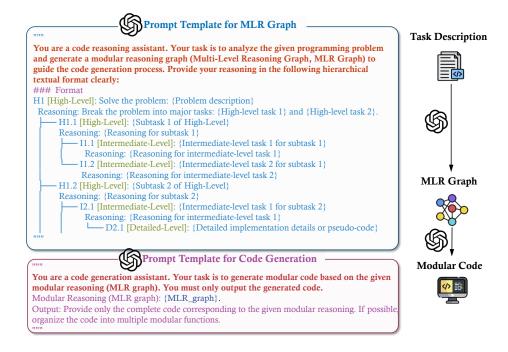


Figure 3: Prompt Templates for the MLR Graph Generation and Modular Code Generation

generation phase, the LLM first generates an MLR graph, categorizing high-level, intermediate-level, and detailed-level designs, according to the description of programming problems. This structured prompting provides guidance during code generation, helps improve modular understanding, and ensures better alignment between reasoning steps and the generated code. Figure 3 illustrates the prompt template (in the blue area) utilized in the MLR graph generation phase.

3.2.1 Multi-Level Reasoning (MLR) Graph. In the MLR graph generation phase, MoT converts the task description analysis into an MLR graph. The graph has a well-defined hierarchy and structure,

which aids the model in understanding task logic and steps while providing effective guidance for subsequent code generation. MLR graphs enable the model to provide modular designs for programming problems by decomposing tasks step by step and embedding a reasoning process.

<u>Task description analysis</u>: Firstly, the LLM extracts key task information from the programming problem, including the goal description, input and output specifications, and related constraints. The goal description typically outlines the core requirements of the programming problem. The LLM identifies relevant features based on the input specifications, such as data type, list length limits, or

condition thresholds. The analysis results form the foundation for modular decomposition.

Modular decomposition: The MLR graph structures task design into three hierarchical levels:

- High-Level: The high-level node designs the primary steps
 of the entire task, including input verification, algorithmic
 logic implementation, and result return. Input validation
 ensures that the input data meets requirements, while the
 algorithmic logic implements the core steps of the task. The
 result return node is responsible for output generation and
 ensuring that the final result meets expectations.
- Intermediate-Level: Intermediate-level nodes further refine the high-level tasks, specifying how each step should be implemented. For example, input validation can be broken down into subtasks such as checking for empty lists and validating data types. Algorithm implementation can be decomposed into defining loop structures and making conditional judgments.
- Detailed-Level: Detailed-level nodes specify detailed implementation operations, such as calculating numerical differences or performing conditional checks.

Each node in an MLR graph is embedded with a reasoning process, which explains the task purpose, decision rationale, and execution strategy:

- Task Purpose: Clarifies the need for the step, such as ensuring input validation to prevent errors in subsequent logic.
- Decision Rationale: Explains the reasoning behind specific choices, for example, using a nested loop to traverse all element combinations.
- Execution Strategy: Describes the operational details of the step, such as determining whether conditions are met or handling boundary cases.

By embedding the reasoning process, the LLMs can gain a better understanding of the design of each node in the MLR graph. In this way, the MLR graph not only delineates the logical structure of task decomposition but also systematically supplies the LLM with the necessary reasoning information for task execution, enhancing its code generation capabilities and logical consistency when processing complex tasks. Note that for simpler programming tasks, LLMs may omit detailed reasoning information for certain nodes and instead provide comprehensive reasoning only for the complex nodes.

3.2.2 An Example. In Figure 4, we present a specific example of an MLR Graph generated from the programming problem description in Figure 2 (partial). The complete MLR graph can be found at our project repository 1 . This figure demonstrates the modular decomposition and step-by-step reasoning process enabled by the MLR Graph for complex programming tasks. The problem is to find the largest sum among the sublists and divide it by K. The MLR graph in Figure 2, which was generated by GPT-4o-mini based on the prompt template given in Figure 3, has three high-level (e.g., "Compute the sum of each sublist"), five intermediate-level (e.g., "Iterate through each sublist"), and five detailed-level nodes (e.g., "Use a for loop to iterate over sublist"), enabling modular reasoning. For

each node, the reasoning consists of three elements: Task Purpose, Decision Rationale, and Execution Strategy. For example, the task purpose of the high-level node "Compute the sum of each sublist" is to calculate the total value of each sublist for subsequent comparison. The decision rationale of the node emphasizes the use of the Python built-in function sum() for efficiency and simplicity. The execution strategy explicitly states that the calculation is performed by iterating over the sublist and invoking the sum() function.

3.3 Code Generation Phase

In the code generation phase, the model leverages the generated MLR graphs to progressively produce code according to the task decomposition structure defined by the nodes. Figure 3 illustrates the prompt templates utilized in the code generation phase. The prompt template in the bottom illustrates how the MLR graph facilitates code generation.

3.3.1 Modular Code Generation based on MLR Graph. The code generation phase builds upon the MLR graph established in the previous phase, enabling the model to effectively complete various components of complex tasks. In this phase, the previously generated MLR graph guides the LLM to generate structured and modular code. The model progressively produces the implementation by following the hierarchical nodes defined in the MLR Graph (from high-level to detailed-level). Each node explicitly corresponds to a specific modular function or defines a code segment, significantly enhancing code modularity and maintainability.

3.3.2 An Example. To better illustrate how the MLR graph guides modular code generation, we present a generated final code based on the MLR graph in Figure 5. The code reflects the hierarchical and modular reasoning defined in the MLR graph.

The high-level task is executed through largest_sum(), which serves as the primary computation function. It is responsible for calling each module sequentially to complete input verification, calculate the maximum sublist sum, and handle the final division operation. The intermediate task further refines the logic, where find_max_sublist_sum() is responsible for processing the input array and computing the maximum sublist sum, while validate_input() ensures the validity of K. The detailed task specifically implements the core computational steps, where compute_sublist_sum() efficiently calculates the sum of a single sublist using Python's built-in sum() function, and divide_max_sum() performs the final division operation, dividing the maximum sublist sum by K to obtain the final result. The entire execution process adheres to the hierarchical design of the MLR graph, ensuring modular reasoning and implementation. The structured guidance provided by the MLR graph can improve the comprehension of the programming problem and lead to better code.

3.4 Overall Algorithm

The MoT algorithm (as shown in Algorithm 1) constructs a hierarchical MLR graph to guide code generation, ensuring logical consistency and correctness. The algorithm consists of two main phases: MLR Graph Generation and Code Generation, leveraging the hierarchical structure to generate code progressively.

 $^{^{1}}https://anonymous.4open.science/r/Modularization_of_Thought/$

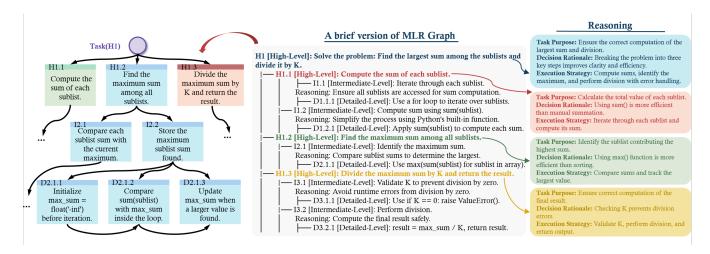


Figure 4: Example of MLR Graph for the problem in Figure 2

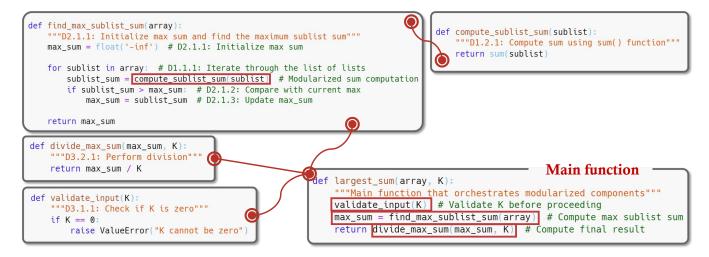


Figure 5: Example of the generated code for the problem in Figure 2

In the MLR Graph Generation phase, the algorithm first parses the task description T and extracts key elements, including the task goal G_T , input-output specifications I_T , and constraints C_T , which serve as the foundation for structured task decomposition. Next, it initializes an MLR graph MLRG to store the hierarchical task structure. Tasks are divided into three types of nodes: High-level task nodes N_T , Intermediate-level task nodes N_M , and Detailed-level task nodes N_B . Each node embeds the MoT reasoning chain to ensure logical consistency.

In the Code Generation phase, the algorithm follows the MLR graph to generate code. First, it initializes the code storage structure C. Then, starting from the high-level task N_T , it sequentially processes intermediate-level tasks N_M and detailed-level tasks N_B , generating code fragments in a structured manner. The generated code follows the MLR graph structure, ensuring logical consistency. Finally, $finalize_code(C)$ integrates all generated code snippets into a complete output C_f .

4 Evaluation

4.1 Research Questions

We evaluate MoT by answering the following research questions (ROs):

- RQ1. How does MoT prompting perform in terms of accuracy compared to baselines?
- RQ2. How effective are the major components of MoT?
- RQ3. What are the cost implications of MoT?

4.2 Datasets

To evaluate MoT, we have conducted extensive experiments on six representative code generation datasets: HumanEval, HumanEval-ET, HumanEval+, MBPP, MBPP-ET, and MBPP+. The details of these datasets are described as follows.

 HumanEval [34] is a benchmark dataset designed to assess the code generation capabilities of large language models.
 It consists of 164 manually crafted Python programming

 ${\bf Algorithm~1}~{\bf Modularization-of-Thought~Prompting~for~Code~Generation}$

```
Require: Task description T
Ensure: Generated code C_f
 1: Phase 1: MLR Graph Generation
 2: G_T, I_T, C_T \leftarrow extract\_task\_elements(T)
                                                       ▶ Extract task
    elements
 3: MLRG \leftarrow initialize\_graph()
 4: for all N_T in generate high level(MLRG, G_T, I_T, C_T) do
        for all N_M in generate_intermediate_level(N_T) do
 5:
            for all N_B in generate_detailed_level(N_M) do
 6:
                embed_reasoning(N_B)
 7:
            end for
 8:
 9:
        end for
10: end for
11: Phase 2: Code Generation
12: C \leftarrow initialize \ code()
   for all N_T in MLRG do
13:
        for all N_M in N_T do
14:
            for all N_B in N_M do
15:
16:
                C \leftarrow generate\_code(N_B, C)
            end for
17:
        end for
18:
19: end for
20: return C_f \leftarrow finalize\_code(C)
```

problems, each accompanied by corresponding test cases to verify the correctness of the generated code.

- MBPP [1] is a dataset comprising diverse Python programming problems. It contains 974 code-generation tasks that cover a wide range of programming scenarios. Each problem is provided with an English requirement, a function signature, and three manually created test cases for validating the generated functions.
- HumanEval-ET and MBPP-ET [38] are extended versions of the original HumanEval and MBPP datasets.
- HumanEval+ and MBPP+ [39] are enhanced versions of HumanEval and MBPP, with the EvalPlus framework augmenting each problem by adding a significantly larger set of test cases—approximately 80 times more than the original dataset.

4.3 Baselines

To evaluate MoT, we consider six typical prompting techniques for comparisons:

- Zero-shot prompting [34] is a method of generating code without utilizing any code examples. The model generates code based solely on problem descriptions.
- Few-shot prompting [34] allows LLMs to choose a few examples for understanding the relationship between problem and code. In our experiments, we adopt the 2-shot setting.
- CoT prompting [7] addresses complex code problems through step-by-step reasoning. When the model approaches a code problem, it first produces a sequence of intermediate steps,

- enhancing the logical coherence and correctness of the generated code.
- Self-planning prompting [9] enables the model to formulate a step-by-step plan prior to code generation. The model creates a comprehensive plan for code generation based on the problem description, which it then executes incrementally.
- SCoT prompting [8] builds upon CoT prompting by leveraging program structures (i.e., sequence, branch, and loop structures) to generate intermediate reasoning steps.
- CodeCoT prompting [10] integrates CoT with self-examination mechanisms. The model improves the accuracy of generated code by producing logically coherent initial code and corresponding test cases, verifying code execution, and iteratively resolving errors as they are identified.

For CoT, SCoT, Self-Planning, and CodeCoT, to achieve fair comparisons, in our experiments, we adopt the prompts used in the respective paper.

4.4 Evaluation Metrics

Following existing work [9, 26–32, 38], we use executable test cases to verify the correctness of the generated code for each programming problem. Then, we employ **Pass@1** [34] and **AvgPassRatio** [40] metrics to assess the performance of LLMs in code generation.

<u>Pass@1</u> measures the functional correctness of the generated code. This metric is used to evaluate the performance of generated code in test cases. Given a programming problem, LLM generates one code instance. The problem is considered solved only if the instance passes all test cases. Pass@1 is the percentage of solved problems out of the total number of problems. The formula is as follows:

Pass@1 :=
$$\mathbb{E}_{\text{Problems}} \left[1 - \frac{n-c}{n} \right]$$
 (1)

<u>AvgPassRatio</u> measures the correctness of the generated code based on its performance across evaluation test cases. Pass@1 focuses on whether the generated code is completely correct in the test case, so we introduce AvgPassRatio to complement it. AvgPassRatio (APR) is calculated by determining the ratio of passed evaluation test cases to the total number of evaluation test cases for each problem and then averaging this ratio across all problems. Larger AvgPassRatio values indicate better code generation performance. Note that in our experiments, APR was not calculated for the MBPP+ dataset as it lacks complete test cases.

4.5 How does MoT prompting perform in terms of accuracy compared to baselines? (RQ1)

1) Setup: To address RQ1, we apply MoT and six baseline techniques to GPT-40-mini [5] and DeepSeek-R1 [6], which demonstrate state-of-the-art performance in code generation among current LLMs. GPT-40-mini is a compact, lightweight version of the GPT model, designed to balance response quality and processing speed. DeepSeek-R1 is an open-source LLM capable of performing high-precision NLP and code generation tasks. In the experiment, we utilize the 671B version of DeepSeek-R1. We used the default temperature parameter provided by the API for both GPT-40-mini

Table 1: Performance	comparison across mi	ultiple datasets and models
Table 1. I citorinance		uitipic datasets and models

Methods	HumanEval		HumanEval+		HumanEval-ET		MBPP		MBPP+	MBPP-ET	
	Pass@1	APR	Pass@1	APR	Pass@1	APR	Pass@1	APR	Pass@1	Pass@1	APR
GPT-4o-mini											
Zero-shot	88.4 (-4.02%)	86.2 (-10.52%)	81.1 (-0.62%)	30.8 (-0.32%)	87.1 (-5.42%)	75.0 (-14.77%)	59.9 (-18.13%)	59.7 (-25.13%)	47.9 (-17.57%)	53.6 (-8.88%)	52.6 (-18.34%)
Few-shot	82.3 (-10.66%)	63.6 (-34.23%)	76.2 (-13.93%)	30.7 (-0.65%)	81.7 (-5.97%)	64.7 (-26.93%)	49.1 (-33.22%)	49.9 (-37.52%)	40.6 (-30.08%)	48.4 (-17.77%)	42.7 (-33.70%)
CoT	87.8 (-4.68%)	79.2 (-18.47%)	82.9 (-5.23%)	29.4 (-4.88%)	87.8 (-0.03%)	86.5 (-1.71%)	61.2 (-3.88%)	62.4 (-21.89%)	48.6 (-6.98%)	54.1 (-3.73%)	53.5 (-16.47%)
Self-planning	87.2 (-5.31%)	90.0 (-7.26%)	79.9 (-9.42%)	30.8 (-0.32%)	87.1 (-4.93%)	74.6 (-15.19%)	52.1 (-29.33%)	54.1 (-32.31%)	42.4 (-27.13%)	48.2 (-18.40%)	46.9 (-27.05%)
SCoT	86.6 (-6.03%)	93.1 (-3.96%)	78.7 (-8.07%)	30.8 (-0.32%)	86.0 (-6.36%)	74.8 (-15.00%)	63.9 (-0.83%)	63.9 (-20.05%)	51.4 (-0.58%)	55.6 (-0.56%)	57.2 (-11.24%)
CodeCoT	83.5 (-9.39%)	84.8 (-12.49%)	73.8 (-10.32%)	30.8 (-0.32%)	82.4 (-8.28%)	81.0 (-8.02%)	55.6 (-13.53%)	56.6 (-29.03%)	40.4 (-19.54%)	53.3 (-0.62%)	48.8 (-24.26%)
MoT	92.1	96.9	83.5	30.9	91.5	88.0	73.9	79.7	58.1	58.9	64.4
DeepSeek-R1											
Zero-shot	93.3 (-1.88%)	93.1 (-3.71%)	87.8 (-6.11%)	31.0 (-0.96%)	92.7 (-1.96%)	80.4 (-3.06%)	69.4 (-7.35%)	72.4 (-7.66%)	57.6 (-3.06%)	64.0 (-5.88%)	58.5 (-9.52%)
Few-shot	84.7 (-10.91%)	66.7 (-30.09%)	79.9 (-10.94%)	31.0 (-0.96%)	84.1 (-0.49%)	75.7 (-8.89%)	69.4 (-7.35%)	69.9 (-0.43%)	57.6 (-3.06%)	64.6 (-5.88%)	57.3 (-2.00%)
CoT	92.6 (-2.71%)	92.6 (-2.91%)	88.2 (-0.21%)	31.0 (-0.96%)	73.5 (-21.53%)	73.5 (-11.30%)	59.9 (-19.02%)	65.4 (-8.31%)	44.4 (-26.22%)	51.9 (-23.38%)	55.4 (-9.71%)
Self-planning	85.4 (-10.24%)	88.3 (-7.35%)	79.3 (-10.45%)	30.8 (-0.96%)	85.3 (-0.21%)	72.3 (-12.83%)	68.4 (-8.57%)	69.2 (-3.03%)	55.4 (-7.06%)	65.5 (-3.75%)	56.4 (-3.51%)
SCoT	84.8 (-10.04%)	81.4 (-14.56%)	79.3 (-10.45%)	30.6 (-2.24%)	84.1 (-0.21%)	72.3 (-12.83%)	57.9 (-22.84%)	60.9 (-15.68%)	46.9 (-19.04%)	61.3 (-5.18%)	55.2 (-4.72%)
CodeCoT	66.5 (-30.89%)	64.9 (-31.82%)	60.4 (-32.85%)	31.3 (0.00%)	65.9 (-28.02%)	58.3 (-29.68%)	69.2 (-6.35%)	88.7 (-1.67%)	56.6 (-2.56%)	64.5 (-8.68%)	74.5 (-5.02%)
MoT	95.1	95.3	88.4	31.3	94.5	82.9	74.9	90.2	60.4	68.0	78.4

and DeepSeek-R1. Subsequently, we measure the effectiveness of each studied prompting technique on 6 widely used benchmarks in terms of Pass@1 and AvgPassRatio metrics. All experiments are conducted on three NVIDIA RTX A800 GPUs with 80GB of memory, and the LLMs are accessed through official APIs.

2) Results: In this section, we compare the performance of the MoT prompting technique across multiple datasets and models against several baseline methods. The evaluation metrics considered include Pass@1 and APR, with results provided in Table 1, respectively.

The results in the Pass@1 metric show that MoT performs well across all datasets, achieving high scores on HumanEval (92.1), HumanEval+ (83.5), HumanEval-ET (91.5), and MBPP (73.9). In comparison, the performance of other prompting techniques is comparatively weaker. For instance, CoT's Pass@1 on HumanEval and MBPP are 87.8 and 61.2, respectively, whereas MoT achieves 92.1 and 73.9 on these datasets, demonstrating clear advantages. Additionally, Self-planning and SCoT do not achieve the performance level of MoT on multiple datasets, with particularly poor results on the MBPP+ and MBPP-ET datasets. While CodeCoT performs well on HumanEval (92.1), it underperforms relative to MoT on MBPP and MBPP-ET, with scores of 55.6 and 58.9, respectively. These results demonstrate that MoT has distinct advantages in generating correct code.

The results in the APR metric show that MoT achieves high APR scores across all datasets, particularly on HumanEval (96.9), HumanEval+ (30.9), and MBPP (79.7). In comparison, APR scores for CoT and SCoT are generally lower, particularly on MBPP and MBPP+. Specifically, the APR of CoT is 79.2 and 62.4, respectively, whereas MoT reaches 96.9 and 79.7 on these datasets, demonstrating MoT's significant advantage in terms of generation quality. Furthermore, CodeCoT's performance in APR is also lower than MoT's, with APR scores of 73.8 and 40.4 on HumanEval+ and MBPP+, respectively, whereas MoT's APR scores are 83.5 and 58.1, further underscoring MoT's advantages in terms of accuracy and quality of generated code. Taken together, MoT demonstrates its ability to generate high-quality code, surpassing other methods including CoT and CodeCoT.

Answer to RQ1: MoT performs well on both Pass@1 and APR metrics, demonstrating its effectiveness across a variety of code generation tasks and models, and surpasses all prompting techniques for code generation.

4.6 How effective are the major components of MoT? (RQ2)

1) Setup: To answer RQ2, we analyze how major components of MoT (as illustrated in Figure 2) affect its effectiveness. We compare the effectiveness of MoT with the following two variants:

- w/o MLR Graph This variant removes the MLR Graph Generation (the graph structure within the red component in Figure 2), which delineates different hierarchical task levels (high-level, intermediate-level, and detailed-level tasks). It retains Modular Decomposition and Code Generation (the yellow component) to generate reasoning chains.
- w/o Modularization: This variant removes the Modular Decomposition component (the red highlighted area within component ① in Figure 2) and the modular Code Generation components (the yellow highlighted area within component ② in Figure 2). Unlike zero-shot or CoT prompting techniques, this variant still utilizes the MLR Graph's hierarchical reasoning structure (high-level, intermediate-level, and detailed-level). Instead of decomposing the task into modular subtasks for separate code generation, the LLM generates the complete final code in a single, monolithic step based on the hierarchical understanding.

2) Results: To assess the effectiveness of MoT's core components, we compare the performance of the whole MoT prompting technique with two variants (w/o MLR Graph and w/o Modularization) on GPT-4o-mini and DeepSeek-R1. The results are presented in Table 2. The results show that MoT outperforms its variants across all datasets, highlighting the critical role of its MLR Graph and Modularization components in enhancing code generation performance.

On HumanEval and MBPP datasets, the Pass@1 score drops significantly when the MLR Graph is removed (w/o MLR Graph). For instance, on GPT-4o-mini, the Pass@1 score for the HumanEval task decreases from 92.1 to 85.4, while on DeepSeek-R1, it drops

Table 2: Performance compa	arison with	different MoT	variants
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Methods	HumanEval		HumanEval+		HumanEval-ET		MBPP		MBPP+	MBPP-ET	
	Pass@1	APR	Pass@1	APR	Pass@1	APR	Pass@1	APR	Pass@1	Pass@1	APR
GPT-40-mini											
w/o MLR Graph	85.4 (-7.27%)	86.5 (-10.74%)	77.4 (-7.31%)	30.8 (-0.32%)	84.3 (-7.87%)	79.0 (-10.23%)	59.9 (-18.94%)	61.9 (-22.29%)	44.6 (-23.25%)	54.4 (-7.64%)	48.6 (-24.48%)
w/o Modularization	82.9 (-9.98%)	79.0 (-18.46%)	78.0 (-6.59%)	30.9 (0.00%)	79.6 (-13.01%)	79.0 (-10.23%)	62.4 (-15.56%)	63.7 (-20.05%)	48.1 (-17.19%)	59.1 (0.34%)	51.6 (-19.81%)
МоТ	92.1	96.9	83.5	30.9	91.5	88.0	73.9	79.7	58.1	58.9	64.4
DeepSeek-R1											
w/o MLR Graph	64.6 (-32.04%)	87.5 (-8.18%)	59.1 (-33.14%)	30.1 (-3.83%)	61.5 (-34.92%)	57.9 (-30.18%)	36.3 (-51.54%)	43.5 (-51.77%)	31.3 (-48.18%)	36.0 (-47.06%)	32.3 (-58.77%)
w/o Modularization	58.5 (-38.45%)	82.4 (-13.53%)	56.1 (-36.54%)	31.0 (-0.96%)	56.8 (-39.89%)	57.7 (-30.39%)	41.6 (-44.47%)	43.1 (-52.22%)	35.3 (-41.56%)	40.5 (-40.44%)	33.1 (-57.78%)
MoT	95.1	95.3	88.4	31.3	94.5	82.9	74.9	90.2	60.4	68.0	78.4

from 95.1 to 64.6, underscoring the key role of the MLR Graph in hierarchical task inference. Additionally, the APR score also declines, further demonstrating the contribution of the MLR Graph.

When Modularization is removed (w/o Modularization), the LLM no longer decomposes programming tasks into modular units but instead adopts a monolithic reasoning approach, significantly impacting task performance. For instance, on GPT-40-mini, the Pass@1 score for HumanEval decreases from 92.1 to 82.9, while the score for the MBPP task drops from 73.9 to 62.4. Similarly, for DeepSeek-R1, the removal of Modularization causes the Pass@1 score for MBPP to decline from 74.9 to 41.6, underscoring the necessity of modular reasoning in code generation.

The complete MoT approach integrates both the MLR Graph and Modularization to achieve optimal performance across all tasks. For instance, on the DeepSeek-R1, MoT attains a Pass@1 score of 95.1 on the HumanEval dataset, exceeding other variants by more than 30%. Similarly, on the MBPP-ET dataset, MoT achieves an APR score of 78.4, significantly outperforming other variants. These results demonstrate that MoT substantially enhances the ability to solve programming tasks through the MLR Graph and modular task decomposition.

Answer to RQ2: Our MoT prompting technique exhibits better performance than its variants, confirming the effectiveness and necessity of its major components.

4.7 What are the cost implications of MoT? (RO3)

1) Setup: The distinction among the HumanEval-related datasets (HumanEval, HumanEval-ET, and HumanEval+), as well as among the MBPP-related datasets (MBPP, MBPP-ET, and MBPP+), is only in the number of test cases, their inputs remain the same. Therefore, we only experimented on HumanEval and MBPP to answer this RQ. We evaluated the cost implications of MoT by running experiments on 164 programming problems from HumanEval and 399 programming problems from MBPP. We calculated the total computational cost required to generate code solutions under different prompting techniques. For accurate cost measurement, we explicitly defined the experimental environment as follows: each problem was solved individually, and the cost was measured based on computational resources consumed, such as token usage.

2) Results: We compared the cost implications of MoT with that of typical prompting techniques, as shown in Table 3.

As shown in Table 3, Zero-shot and few-shot prompting techniques have notably lower computational costs compared to other prompting techniques. Specifically, zero-shot has the lowest Intoken consumption, while few-shot achieves the lowest overall cost due to its lowest Out-Token consumption. Given the cost of an output token is typically much higher than that of an input token, few-shot has a lower cost than Zero-shot. Although these two simple prompting techniques have low computational costs, they typically have inferior performance.

The results in Table 3 show that MoT demonstrates superior efficiency and lower computational cost compared to other typical prompting techniques. The cost of MoT on the HumanEval and MBPP datasets is 0.0044 and 0.0042, respectively, making it a more cost-efficient method. For instance, the cost of CoT is 0.0047 and 0.0044, which are 6.82% and 4.76% higher than those of MoT, while its In-token and Out-token consumption also increase by 0.60% / 4.12% (HumanEval) and 3.41% / 2.61% (MBPP), respectively. In addition, both Self-planning and SCoT exhibit significantly higher costs compared to MoT. The cost of Self-planning increases by 40.91% on HumanEval and 40.48% on MBPP, with In-token and Out-token consumption rising by 4.06% / 28.84% (HumanEval) and 17.27% / 27.61% (MBPP), respectively. Similarly, SCoT experiences a substantial increase in In-token and Out-token consumption, leading to higher computational costs. Notably, the cost of CodeCoT on the HumanEval and MBPP datasets reaches 0.0071 and 0.0050, respectively, which are 61.36% and 19.05% higher than those of MoT. At the same time, its Out-token consumption increases significantly by 51.74% and 17.49%, further reinforcing MoT's advantage in reducing the computational cost. These results demonstrate that MoT significantly reduces the cost of solving programming problems by minimizing additional generation, such as test case generation in CodeCoT.

Compared with existing methods, MoT (as shown in Figure 6) has the lowest time cost, with an average generation time of 5 seconds, while CodeCoT takes 13 seconds, SCoT takes 9 seconds, and Self-planning takes 6 seconds. Unlike techniques such as CodeCoT, MoT does not require generating test cases, executing code, or iterative generation. Reducing unnecessary steps leads to a more efficient process, enabling MoT to achieve improved performance without compromising effectiveness.

Table 3: Performance comparison on GPT-40-mini across multiple datasets and models (Cost, Token)

Methods	Cost (\$)	HumanEval In-token	Out-Token	Cost (\$)	Out-Token	
Zero-shot	0.0028(-36.36%↓)	119.1 (-76.26%↓)	357.6 (26.62%↑)	0.0025 (-40.48%↓)	45.1 (-90.85 %↓)	340.5(-10.96%↓)
Few-shot	0.0016 (-63.64% \(\psi \)	374.6(-25.28%↓)	58.0 (-79.45%↓)	0.0022 (-47.62% \(\psi \)	578.8 (17.26%↑)	157.0 (-58.92% \(\psi \)
CoT	0.0047 (6.82%↑)	504.3 (0.60% [†])	293.9 (4.12% 1)	$0.0044 (4.76\%\uparrow)$	510.4 (3.41%)	390.5 (2.61% [†])
Self-planning	0.0062 (40.91%↑)	521.6 (4.06%↑)	364.1 (28.84%†)	0.0059 (40.48%↑)	578.9 (17.27%†)	488.1 (27.61%↑)
SCoT	0.0058 (31.82%↑)	508.8 (1.49% 1)	384.2 (36.16%↑)	0.0052 (23.81%†)	559.7 (13.37%†)	479.6 (25.46% 1)
CodeCoT	0.0071 (61.36%†)	535.5 (6.82%↑)	428.7 (51.74%†)	0.0050 (19.05%†)	534.0 (8.17%↑)	449.1 (17.49%↑)
MoT	0.0044	501.3	282.4	0.0042	493.6	382.4

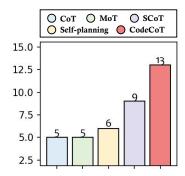


Figure 6: Comparison of Average Generation Time for Different Prompt Techniques on the HumanEval Dataset

Answer to RQ3: Based on these results, we conclude that MoT offers an efficient solution to achieve better performance, which incurs significantly lower cost than other prompting methods except simple zero-shot and few-shot.

5 Discussion

5.1 Why is MoT Effective?

MoT constructs an MLR graph to delineate different levels of tasks, such as high-level, intermediate-level, and detailed-level tasks. This modular approach provides the LLM with a clear hierarchical framework during the reasoning process. By explicitly defining task boundaries and dependencies, the MLR graph guides the model to systematically address each module, thereby mitigating ambiguity and promoting logical clarity. Unlike traditional linear prompting methods that rely on sequential reasoning without explicit structure, MoT significantly reduces the potential for context confusion or unclear dependencies between steps. Moreover, by decomposing complex problems into modular sub-tasks, MoT reduces cognitive complexity and enables the model to more accurately and efficiently manage each sub-task. This modular reasoning not only improves the overall coherence of the generated code but also enhances maintainability and scalability, making it easier to debug, test, and extend the generated solutions. Consequently, MoT demonstrates substantial improvements in code generation quality when handling sophisticated programming problems.

To illustrate the effectiveness of the MLR Graph in modular code generation, we analyze the specific programming task shown in

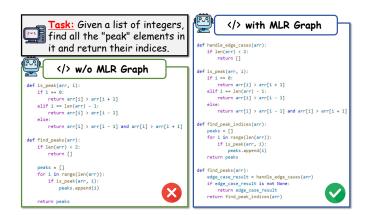


Figure 7: An example for the effectiveness of MLR Graph

Figure 7. The task requires identifying all "peak" elements in a given list of integers and returning their indices. The left side of the figure displays the code generated without MLR graph guidance, while the right side presents the code generated with MLR graph guidance. From the figure, it is evident that the right-side implementation, guided by the MLR graph, follows a well-structured and modular approach. It first handles edge cases (when the list length is less than 2), then separately defines two key logical components: one for determining whether an element is a peak (is peak) and another for finding the indices of all peak elements (find_peak_indices). Finally, the main function find_peaks integrates these modular components to complete the task. This modularization improves both the readability and maintainability of the generated code. The code on the left, which does not utilize MLR graph, lacks explicit handling for boundary cases (e.g., when the array length is less than 2, an index out-of-bounds error may occur). Additionally, its reasoning is monolithic, reducing both readability and robustness. Consequently, this implementation is prone to logical flaws and incomplete boundary case handling, making it more susceptible to unexpected errors. This example demonstrates that the MLR graph effectively guides LLMs in modular task decomposition and modular code generation. By leveraging this modular approach, MLR Graph enhances code quality and improves readability.

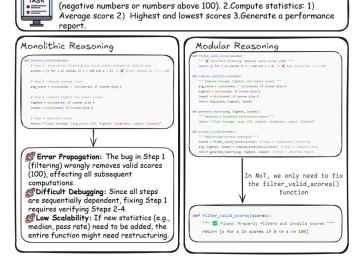
5.2 MoT for Code Maintainability

MoT is aligned with good practices in software engineering, such as information hiding and modular decomposition, which have been

shown to enhance system flexibility, maintainability, and scalability [15, 16]. By incorporating these principles into the reasoning process of LLMs, MoT employs a modular reasoning approach to decompose complex code generation tasks into multiple independent yet interrelated modules, enabling each reasoning step to be optimized, iterated, and adjusted independently. Unlike CoT, which follows a monolithic reasoning process where all steps are highly coupled — making local error correction challenging. MoT allows for localized adjustments to reasoning steps, thereby reducing error propagation.

We provide an illustrative example in Figure 8 to demonstrate the advantages of Modularized Reasoning compared to traditional monolithic reasoning. In traditional monolithic reasoning approaches (left side of Figure 8), all logic is encapsulated within a single module or function (e.g., the function *process_scores()*). This structure inherently causes any error within an intermediate step, such as incorrectly filtering valid scores, to propagate through subsequent computations. As a result, identifying the origin of such errors becomes cumbersome, requiring verification of multiple sequentially dependent steps. Moreover, extending such monolithic functions to accommodate new statistics or additional logic becomes challenging, reducing scalability and maintainability.

In contrast, as illustrated on the right side of Figure 8, the Modular Reasoning (MoT) decomposes the task into multiple independent yet interrelated modules. Each module, such as <code>filter_valid_scores()</code>, <code>compute_statistics()</code>, and <code>generate_report()</code>, is clearly defined and encapsulated with specific functionality. Consequently, debugging and correcting errors—like the improper filtering step—become simpler and more targeted, requiring modification of only the relevant module (<code>filter_valid_scores()</code>). Furthermore, adding new functionalities or statistics can be achieved by introducing or updating individual modules without necessitating substantial restructuring of the overall code. Thus, modular reasoning significantly enhances the efficiency, scalability, and reliability of the generated code.



Given a list of student scores, we need to: 1. Filter out invalid scores

Figure 8: An example for MoT for Code Maintainability

5.3 Threats to Validty

The main limitations of our work lie in the following two aspects: Firstly, due to the randomness involved in LLMs, different outputs may be provided with each generation. As a result, even with identical input, MoT may yield different outputs, which can impact the accuracy and consistency of the final code generation. To solve this issue, we conduct extensive experiments to minimize influences caused by randomness involved in LLMs, such as performing repeated experiments on various benchmarks. This approach ensures consistent results in most cases and helps reduce unusual fluctuations in individual tests by evaluating averages.

Secondly, our current analysis primarily focuses on Python code generation, while the characteristics of other programming languages may not be fully explored. Different programming languages have distinct syntax and structures, which may result in varying effectiveness and performance of MoT. To address this limitation, we selected Python, a widely used and representative language, for the experiments. However, the modularization concept of MoT is applicable to most programming languages. In our future work, we plan to conduct more comprehensive evaluations across a broader range of programming tasks such as system programming and web development to further explore the adaptability and performance of MoT.

6 Conclusion

In this paper, we propose a novel prompting technique MoT to improve the code generation performance of LLMs. Different from the existing prompting techniques, MoT incorporates the modularization principles into the reasoning process. It introduces a novel Multi-Level Reasoning (MLR) graph to enhance modular understanding and ensure alignment between reasoning and the generated code by hierarchically organizing reasoning steps with its modular structure. We conducted an extensive study with two advanced LLMs on six widely-used benchmarks. The results confirm the superiority of MoT over state-of-the-art prompting techniques.

Our source code, experimental data, and concrete examples of prompts and generated code are available at https://anonymous.4open.science/r/Modularization of Thought/.

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