Constrained Decoding of Diffusion LLMs with Context-Free Grammars

Niels Mündler, Jasper Dekoninck, Martin Vechev

Department of Computer Science ETH Zurich, Switzerland {niels.muendler,jasper.dekoninck,martin.vechev}@inf.ethz.ch

https://constrained-diffusion.ai
https://github.com/eth-sri/constrained-diffusion

Abstract

Large language models (LLMs) have shown promising performance across diverse domains. Many practical applications of LLMs, such as code completion and structured data extraction, require adherence to syntactic constraints specified by a formal language. Yet, due to their probabilistic nature, LLM output is not guaranteed to adhere to such formal languages. Prior work has proposed constrained decoding as a means to restrict LLM generation to particular formal languages. However, existing works are not applicable to the emerging paradigm of diffusion LLMs, when used in practical scenarios such as the generation of formally correct C++ or JSON output. In this paper we address this challenge and present the first constrained decoding method for diffusion models, one that can handle formal languages captured by context-free grammars. We begin by reducing constrained decoding to the more general additive infilling problem, which asks whether a partial output can be completed to a valid word in the target language. This problem also naturally subsumes the previously unaddressed multiregion infilling constrained decoding. We then reduce this problem to the task of deciding whether the intersection of the target language and a regular language is empty and present an efficient algorithm to solve it for context-free languages. Empirical results on various applications, such as C++ code infilling and structured data extraction in JSON, demonstrate that our method achieves near-perfect syntactic correctness while consistently preserving or improving functional correctness. Importantly, our efficiency optimizations ensure that the computational overhead remains practical.

1 Introduction

Large language models (LLMs) have recently achieved promising performance across a wide range of tasks [18, 39]. Due to their capabilities in code synthesis, they achieve impressive scores on diverse code benchmarks [8, 21, 24, 51] and are integrated into developer workflows as programming copilots [16, 48]. Further, they are used for processing information into machine-readable formats, with commercial providers offering restricting output to JSON or context-free grammars [2, 40]. Despite these successes, LLMs are inherently probabilistic and offer no guarantees that their generated output will be syntactically valid, providing an inherent limitation for LLM users.

Prior constrained decoding is limited A promising approach that mitigates this limitation is constrained decoding [6, 31, 42, 50]. This technique leverages the formal grammar of a target language to guide the generation process, ensuring that the output remains within the language's

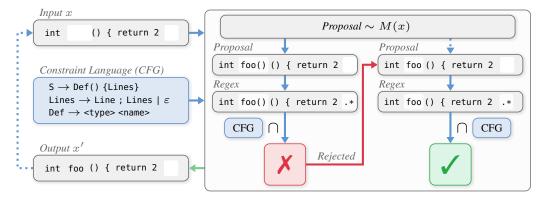


Figure 1: An overview of our approach. In each step, the input consists of a partial text x with arbitrarily many infilling regions and a context-free grammar (CFG) specifying formal constraints. During decoding, we sample a proposal to insert a token in one of the regions from a model M. Our method then intersects the CFG with the regular language containing all possible completions of the updated input x. If the proposal intersection is empty, the proposal is rejected and a new proposal is sampled. Otherwise, it is accepted and the decoding continues with the updated partial output x'. In the example, the invalid proposal "foo()" is rejected and "foo" accepted instead.

bounds. Constrained decoding leverages parsing and validation of the generated output in lockstep with the incremental generation process, allowing the model to avoid invalid continuations without restarting inference.

Most constrained decoding methods restrict left-to-right prefix completion to context-free grammars (CFGs). This setting is relevant, as prefix completion is a common LLM generation settings, and CFGs capture the syntax of common programming languages and popular data formats, like C++ and JSON [9, 25]. Melcer et al. [31] extend constrained decoding for single-region infilling, supporting completions between a fixed prefix and suffix. Suresh et al. [47] constrain diffusion LLMs to regular languages, but can thus not handle important applications, such as C++ or JSON. No prior work supports multi-region infilling (MRI) or diffusion LLM (DLM) constraining with CFGs.

This work: Constrained decoding for MRI and DLMs In this work, we present a generalized method for constrained decoding of multi-region infilling and out-of-order generation. We first generalize the formal framework of constrained decoding by adapting the standard constrained decoding algorithm to unordered updates of a partial output with arbitrarily many infilling regions, capturing both MRI and DLM. The decoding process is illustrated in Figure 1. The model iteratively generates proposals to insert a token in a specific location of the partial output. We verify that this proposal is valid by intersecting the target language's CFG with the language of all possible completions of the partial output. This intersection is non-empty if and only if a valid completion exists.

A key technical challenge to this approach is to efficiently determine the emptiness of the language intersection. We first show that the language of possible completions is a regular language, enabling standard formal language operations to generate the intersection language. We then address the cubic size of the intersection language by applying optimizations for size reduction, such as employing a custom normal form. Further, we perform an implicit search over the intersection language to avoid generating the entire language, and all non-generating symbols in particular.

Experimentally confirmed consistent improvements Our experiments demonstrate a substantial improvement in the reliability of formal language adherence across all evaluated settings. Specifically, the algorithm guarantees valid completions in all settings, up to timeouts by the model. Additionally, it improves functional correctness by up to 7%. Importantly, our approach incurs only modest overhead on tested models with 7B parameters, with inference time less than doubling on average, enabling practical usage even in the most complex settings.

Key contributions Our three key contributions are; (i) a generalization of the formal constrained decoding framework for MRI and DLM settings, (ii) a novel constrained decoding algorithm for these settings, and (iii) an extensive evaluation of our method using state-of-the-art open-weight infilling

and diffusion LLMs, demonstrating consistent improvements in syntactic and functional correctness on C++ code generation, JSON schema extraction, and chemical molecule description.

2 Background

We outline the necessary background relevant to this work, including generation paradigms with LLMs, constrained decoding, and the relevant properties of regular and context-free languages.

2.1 LLM Generation Paradigms

We focus on four generation settings with LLMs illustrated in Figure 2a. The first three approaches are commonly used with autoregressive models and generate outputs left-to-right.

PRE, FIM and MRI First, Prefix (PRE) generation completes a fixed prefix, commonly used for synthesizing text or code from scratch. Second, Fill-In-the-Middle (FIM) completes text between prefix and suffix, widely used for code completion assistants [16, 22]. Third, Multi-Region Infilling (MRI) generalizes FIM with multiple fixed snippets, interleaved by infilling regions. This enables more flexible editing and structured completion tasks, such as infilling multiple function bodies.

Generation with DLMs Diffusion Language Models (DLMs) [36, 55] iteratively insert tokens into an initially empty or partially filled sequence (x_1, x_2, \ldots, x_n) where each x_i is either a token from the vocabulary V or a mask \bot . At each step, the model outputs an index k of a mask token, i.e., $x_k = \bot$, and a token $t \in V$ to produce the updated sequence $(x_1, \ldots, x_{k-1}, t, x_{k+1}, \ldots, x_n)$. This process continues until no masks remain. In the example in Figure 2a, the model would first generate the return statement (1), then the function name (2), and finally the return value (3).

Constrained generation Constrained generation restricts the model to produce outputs that conform to predefined syntactic or structural rules, ensuring syntactically valid code or adherence to structural patterns [42]. Formally, the model must generate an output $w \in L$, where L is a formal language defining admissible programs for the given task. Constrained decoding is typically implemented by restricting the model's output space at each step, either by masking invalid tokens [50] or by sampling and rejecting invalid outputs [31]. Most prior works apply these techniques to the PRE setting and CFGs [6, 42, 50], with some extensions to FIM and context-sensitive features [31, 34]. Suresh et al. [47] constrain DLMs specifically, but only to regular languages. To our knowledge, constrained decoding with CFGs has not yet been applied to the MRI or DLM paradigms.

2.2 Regular and Context-Free Languages

We briefly outline the properties and notation of regular and context-free languages that are relevant to our method. We provide a more detailed introduction in Appendix A.

Regular Languages A regular language is a set of strings that can be described by a deterministic finite automaton (DFA). A DFA is defined as a tuple $(Q, \Sigma, \delta, q_0, F)$, where: (1) Q is a finite set of states, (2) Σ is a finite alphabet of symbols, (3) $\delta: Q \times \Sigma \to Q$ is a transition function that maps a state and an input symbol to the next state, (4) $q_0 \in Q$ is the initial state, and (5) $F \subseteq Q$ is the set of accepting states. The language of a DFA consists of those strings that transition the automaton from the initial to an accepting state through the transition function. Figure 2b depicts a non-deterministic finite automaton (NFA), which additionally allows multiple next states for the same state and symbol and traversing ε -transitions without consuming a symbol. Every NFA is equivalent to some DFA.

Context-Free Languages Context-free languages (CFLs) are a superset of regular languages, including languages that enforce recursive structures, such as balanced parentheses or nested control statements. They can be described by context-free grammars (CFGs). A CFG is a tuple (V, Σ, P, S) , where: (1) V is a finite set of nonterminals, (2) Σ is a finite set of terminals (with $V \cap \Sigma = \emptyset$), (3) P is a set of productions $A \to \alpha$, with $A \in V$ and $\alpha \in (V \cup \Sigma)^*$, and (4) $S \in V$ is the start symbol. The language is defined as all strings generated by the following procedure: Starting with S, apply a rule $A \to \alpha$ from P to replace nonterminal S0 with S1, until the result contains only terminals.

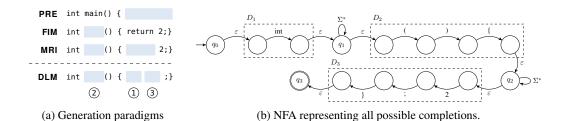


Figure 2: We consider three left-to-right (PRE, FIM, MRI) and one out-of-order (DLM) generation paradigms (a). The NFA in (b) describes the language of all additive completions for the MRI task.

3 Constrained Decoding for Infilling and Diffusion

In this section, we first formally define the decision problem that enables MRI and DLM generation settings, and then introduce our algorithm for efficiently deciding the problem. We then provide adapted constrained decoding algorithms for MRI and DLM.

3.1 The Constrained Infilling Problem

Constrained decoding with infilling First, let us define a partial output \mathbf{x} as a sequence of strings $x_1, x_2, \ldots, x_n \in \Sigma^*$ with arbitrary sized infilling regions \Box , i.e., $\mathbf{x} = x_1 \Box x_2 \ldots \Box x_n$. In constrained decoding, sketched in Algorithm 1, we complete \mathbf{x} using model M and target language L. We iteratively sample an updated proposal and partial output \mathbf{x}' from a model (Lines 1 and 2). All proposals modify the input additively, meaning they either insert a string into existing regions, e.g., insert b into $a \Box c$ resulting in $a \Box b \Box c$, or remove a region by merging adjacent strings,

e.g., creating $a \square bc$ from the previous output. If \mathbf{x}' completes the last infilling region and is valid with respect to L, we return the final updated output (Lines 3 and 4). Otherwise, we check whether the updated output can be completed into a valid completion according to L (Line 5). If so, we apply the proposal and update \mathbf{x} (Line 6). Otherwise, we reject the proposal and remove it from the model distribution (Line 8). After that, the process continues. Because no proposal removes parts of the output, and the output is guaranteed to be completable, Algorithm 1 always terminates.

Deciding proposal validity To enable constraining additive generation, we need an incremental verifier COMPLETABLE to determine whether the regions in a partial output can be filled to produce a valid output in L. We formalize the decision problem solved by COMPLETABLE as follows:

Definition 1 (Constrained infilling problem). For a language L, partial output $\mathbf{x} = x_1 \Box x_2 \ldots \Box x_n$ with $x_i \in \Sigma^*$ and \Box denoting infilling regions, the constrained infilling problem is whether there exists a list of n-1 words $\mathbf{y} = (y_1, \ldots, y_{n-1})$ such that $w = x_1 \cdot y_1 \cdot x_2 \cdot \ldots \cdot y_{n-1} \cdot x_n$ is in L.

Thus, with the incremental verifier deciding the constrained decision problem, we have effectively reduced constrained decoding with infilling to the constrained infilling problem.

Applications of the constrained infilling problem We can reduce constrained decoding for PRE, FIM, MRI, and DLM generation to the constrained infilling problem. PRE for a given prefix p is the special case where $\mathbf{x} = p \square \varepsilon$. FIM with prefix p and suffix s is the special case where $\mathbf{x} = p \square s$. For MRI, the list of words corresponds to the list of fixed snippets, with infilling regions in between. For the DLM setting, we add implicit ε tokens at the beginning and end of the partially filled sequence and then merge all consecutive non-mask tokens to build \mathbf{x} . For example, the sequence $(a, \bot, \bot, b, c, \bot)$ becomes $\mathbf{x} = a \square bc \square \varepsilon$. Note that, similar to prior work [6, 50], we slightly overapproximate in these representations, by allowing infillings of arbitrary size where there might be practical limitations to the number of tokens to insert for an LLM. We discuss this in more detail in Appendix E.

3.2 Deciding the Constrained Infilling Problem Efficiently

Overview We now give a brief overview of how to solve the constrained infilling problem efficiently. The problem is determined by two separate constraints: (1) the structural constraints on the output, described by the context-free language L, and (2) all possible completions of the partial output \mathbf{x} , which forms a language $C_{\mathbf{x}}$. For example, L could be the language of syntactically valid C++ programs, and $C_{\mathbf{x}}$ the language of completions of partial program $\mathbf{x} = \mathsf{int} \square() \{ \square 2; \}$. The infilling problem is answered positively if and only if the intersection $L_{\cap} = L \cap C_{\mathbf{x}}$ is not empty, i.e., some infilling of the partial output exists to generate a valid word in L. We will show that $C_{\mathbf{x}}$ is a regular language that we can describe with a simple DFA, and that L_{\cap} can be described by a context-free grammar, which we can construct from L's grammar and $C_{\mathbf{x}}$'s DFA. The constrained infilling problem is then reduced to checking whether L_{\cap} is empty, for which we design an efficient algorithm. In the example, a word in the intersection language is int main() {return 2;}.

Note that the algorithm designed in this section operates on language terminals, which may not align with LLM tokens. In Appendix C, we demonstrate how to apply the algorithm to partial outputs generated by LLMs and how we can resolve the various issues that arise from this mismatch.

Constructing the regular language The language $C_{\mathbf{x}}$ of all possible completions of $\mathbf{x} = x_1 \square \ldots \square x_n$ contains all words that start with x_1 , end with x_n , and contain the strings x_i $(1 \le i \le n)$ in the correct order, with arbitrary symbols in between. We now construct an NFA that accepts $C_{\mathbf{x}}$, proving it is regular. We first construct the automata D_i , which accept exactly x_i . Then, we concatenate D_i with an additional state q_i that accepts any string in Σ^* , i.e., $\delta(q_i, \sigma) = q_i$ for all $\sigma \in \Sigma$. For the concatenation, we add an ε -edge from the accepting states of D_i to D_i and from D_i to the start state of D_{i+1} . We then transform the NFA into a minimal DFA using a standard method [20]. A visualization for the prior example is shown in Figure 2b.

Constructing the intersection language We leverage the well-established facts that (a) the intersection L_{\cap} of CFL L and regular language $C_{\mathbf{x}}$ is a CFL, whose grammar can be constructed from L's grammar G and $G_{\mathbf{x}}$'s DFA, and (b) that the emptiness of a CFL can be checked in time polynomial to the size of the grammar [14, 20]. However, following the standard construction, the resulting grammar $G_{\cap} = (V_{\cap}, \Sigma, P_{\cap}, S_{\cap})$ will have a cubic blowup in nonterminals and productions, with $|V_{\cap}| \in O(|V||Q|^2)$ and $|P_{\cap}| \in O(|P||Q|^3 + |P||Q|^2|\Sigma|)$ [4, 14]. In order to ensure the practicality of our method, we need to reduce the size of and computations on the intersection grammar.

Efficient normalization The standard intersection algorithms require G to be transformed into Chomsky normal form, which only allows rules of the form $A \to BC$ or $A \to a$, where $A, B, C \in V$ and $a \in \Sigma$ [20]. The resulting grammar may have a quadratic increase in the number of production rules [28]. To avoid this blowup, we extend the standard construction to support CFGs in $C2F^{+\varepsilon}$, a normal form that additionally allows productions of the form $A \to \varepsilon$ and $A \to B$. This normal form can be obtained with only a linear increase in production rules [28]. In Appendix B.1, we describe several further optimizations to reduce the size of the normalized CFG of G. Our adaptations to the standard intersection algorithm and a proof of its correctness are provided in Appendix B.2.

Avoiding nongenerating nonterminals A naive algorithm to check whether the intersection language L_{\cap} is empty would explore the entire grammar. However, many of the nonterminals and productions in the intersection grammar are not *generating*, i.e., there are many symbols A for which there does not exist a sequence of production applications $A \to \cdots \to w$ such that $w \in \Sigma^*$ consists only of terminals [35]. We therefore adapt an efficient bottom-up search by D.W. [10] to $C2F^{+\varepsilon}$ that by construction only expands on generating nonterminals, and decides emptiness in time linear to the number of nonterminals and productions in the language. The algorithm starts with the symbols that generate terminals or empty strings directly, i.e., all A with productions $A \to \sigma$ and $A \to \varepsilon$. It marks these symbols as generating and inserts them into a queue. Next, for each symbol X in the queue, it checks whether some production has X on the right-hand side (i.e., either $A \to XC$, $A \to BX$ or $A \to X$), and optionally checks whether the other symbol $(B \to C)$ in the production was previously marked as generating. If so, we mark A as generating as well and add it to the queue. As soon as we mark the start symbol S, we conclude that the language is non-empty, since there must exist a sequence of production applications $S \to \cdots \to w$, which implies $w \in L$.

Searching through the implicit intersection language To further improve performance, we conduct the search outlined above implicitly by leveraging the structure of the intersection language. All symbols in the intersection language have the form ${}^p\vec{A}^q$ for $p,q\in\Sigma$ and $A\in V$. All production

rules in the intersection grammar are directly derived from corresponding rules in the original CFG. Specifically, all rules of the form $\overset{p}{A}\overset{q}{\to}\varepsilon$ and $\overset{p}{A}\overset{q}{\to}\sigma$ are based on corresponding rules $A\to\varepsilon$ and $A\to\sigma$ in the original grammar without further dependencies, allowing us to iterate over directly generating symbols without constructing the remaining grammar. Further, all other rules are of the form $\overset{p}{A}\overset{q}{\to}\overset{p}{B}\overset{r}{C}\overset{q}{\to}$ and $\overset{p}{A}\overset{q}{\to}\overset{p}{B}\overset{q}{\to}$ based on original productions $A\to BC$ and $A\to B$, for all $p,q,r\in Q$. This enables enumerating all such rules for a given $\overset{p}{B}\overset{r}{,}\overset{r}{C}\overset{q}{\to}$ or $\overset{p}{B}\overset{q}{\to}$ on the fly. We present the corresponding pseudo-code and additional explanations in Appendix B.3.

Sampling a valid completion from the intersection language The algorithm presented above can be easily extended to return a valid completion from the intersection language. To achieve this, we modify the algorithm to track the applied rules that mark each symbol as generating. This sketches a parse tree for some word w in the intersection language. We then traverse the terminals at the leaf nodes of this tree from left to right to reconstruct a valid completion in the intersection language. We use this completion when the LLM is unable to generate a valid proposal after a fixed number of rejected proposals. Since the algorithm leverages the results from the prior emptiness search, it can be run at no additional cost. We observe that only 0.7% of valid completions do not appear in the first 50 selected LLM proposals. Thus, we can significantly speed up the sampling process without losing performance by inserting a randomly sampled valid completion after k rejected proposals. In our experiments, we set k to 100 to ensure we do not miss any valid completions.

4 Experimental Evaluation

We evaluate our method across a range of tasks and models, first in the FIM and MRI settings, and then in DLM, demonstrating improvements in both syntactic and functional correctness. We provide further experimental details, ablate DLM diffusion steps, and provide a case study in Appendix D.

4.1 Experimental Setup

Metrics We compute two main metrics to evaluate the effectiveness of our method. First, we determine the percentage of syntactically correct completions (Syntax), which indicates how many of the obtained completions adhere to the specified grammar. We also measure functional correctness (Functional) by either comparing the sample to a golden solution, or by reporting the percentage of solutions that pass all test cases, pass@1, depending on the dataset. All results are averaged over four independent runs with different seeds. We compute confidence intervals at 95%, **boldface** the best method, and <u>underline</u> all methods over which the increase is not significant. The usual size of the confidence interval is 1% to 2%.

Compared methods We run unconstrained LLM sampling, reported as Vanilla (*Van.*). We also run constrained decoding with our method. We abort generation if decoding exceeds the maximum number of 256 tokens, or rejects 100 proposals. In *Con.*⁻ we report aborted instances as syntactically and functionally invalid. In *Con.*, we complete aborted instances by sampling a valid completion from the intersection language. Remaining errors are due to model timeouts.

4.2 Fill-In-the-Middle and Multi-Region-Infilling

Models We compare the performance of five recent open-weight infilling models, including STAR-CODER2 7B [30], CODEGEMMA 7B [56], and the DEEPSEEK CODER Family [19], covering 7B parameter models from three distinct model families and model sizes from 1.3B to 33B.

Tasks and benchmarks Infilling is commonly used to complete partial code [5, 13]. We therefore evaluate our method on the C++ translation of the HumanEval dataset [8, 57], containing 164 diverse basic coding tasks. Similar to Bavarian et al. [5], we transform the dataset into an infilling task by removing random spans from the human-written reference implementation. We evaluate up to three removed spans, resulting in 1-MRI, 2-MRI, and 3-MRI. To guide the model, we design a CFG for the relevant part of the C++ syntax. We report adherence to this CFG as syntactic correctness. Functional correctness is measured by computing the pass@1 score on provided test cases [7].

Syntactic correctness As can be seen in Table 1, our method increases syntactic correctness significantly across all models and numbers of infilling regions. Deriving a valid completion from

Table 1: Our method consistently improves the percentage of syntactically and functionally correct infillings for varying numbers of regions in MRI under standard decoding (Van.), constrained decoding (Con.⁻), and completing partially completed outputs (Con.).

			1-mri			2-mri			3-mri	
	Model	Van.	Con	Con.	Van.	Con	Con.	Van.	Con	Con.
Syntax	STARCODER2 7B	88.2	95.0	98.9	55.4	77.7	96.3	24.5	57.2	88.3
	CODEGEMMA 7B	92.5	97.2	100.0	61.5	85.6	99.0	29.9	66.4	96.0
	DEEPSEEK C. 1.3B	86.5	91.7	98.7	51.5	72.9	93.1	22.7	47.7	83.0
	DEEPSEEK C. 6.7B	93.9	98.3	100.0	62.0	84.0	97.3	32.9	64.9	94.6
	DEEPSEEK C. 33B	93.1	97.6	100.0	66.3	86.5	97.8	36.4	67.8	93.5
Functional	STARCODER2 7B	53.8	56.1	56.3	20.5	23.7	24.2	7.5	10.3	11.0
	CODEGEMMA 7B	57.1	59.6	59.6	24.8	<u>29.0</u>	29.2	8.7	12.6	12.8
	DEEPSEEK C. 1.3B	<u>46.5</u>	46.4	47.2	16.1	18.4	19.2	4.9	5.4	6.5
	DEEPSEEK C. 6.7B	64.8	67.1	67.3	29.8	<u>32.7</u>	33.2	11.9	13.5	13.5
	DEEPSEEK C. 33B	69.8	71.2	71.4	29.8	<u>34.0</u>	34.3	12.6	14.3	15.4

the intersection language (Con.) recovers a syntactically valid completion in 95.8% of instances. Constraints increase syntactic correctness without completions (Con. $^-$) more for code with multiple regions, where models struggle more, achieving an absolute increase of 5.2%, 22.5%, and 31.5% for 1-MRI, 2-MRI, and 3-MRI, respectively. These improvements are consistent across model families and sizes, ranging between 17% and 21% per model.

Functional correctness In the lower half of Table 1, we observe that constraining (Con. $^-$) consistently increases functional correctness, on average by 2.4%, and additionally sampling valid completions (Con.) improves the increase to 2.8%. This is expected, as syntactically incorrect completions can not be functionally correct and are effectively prevented by our method.

Runtime overhead We compare the time per token between constrained and vanilla decoding. The median runtime overhead of constrained decoding is 125%, where the overhead on the small DEEPSEEK CODER 1.3B is higher (320%) than on the 7B models (100%) and DEEPSEEK CODER 33B (20%). Moreover, more infilling regions also increase the median overhead, growing from 67% on 1-MRI to 205% on 3-MRI.

4.3 Diffusion Language Models

Models We evaluate our method on the instruction-tuned versions of four state-of-the-art diffusion language models, LLADA 8B [36], DREAM 7B [55], DREAMCODER 7B [54] and DIFFUCODER 7B [17]. We run all models with 32 steps on 256 tokens and with a temperature of 0.2.

Tasks and benchmarks As DLMs are generic text generation models with many different applications, we design three distinct and diverse tasks:

- C++ Based on the dataset used in §4.2, the model should generate the entire function specified in natural language [8, 57].
- JSON The model should extract relevant information from natural language input, adhering to a JSON-Schema specification [37].
- SMILES The model should write down a chemical molecule described in natural language in the SMILES specification language [52].

For SMILES and JSON we generate synthetic benchmarks using GEMINI-2.5-PRO [18] with verification to ensure that the generated samples are correct and solvable, resulting in 167 and 272 instances respectively. More details about the dataset generation procedure can be found in Appendix D.3.

We implement the syntax of each language as a CFG and use it to enforce and evaluate the syntactic correctness of the generated output. For C++, we measure functional correctness using pass@1 as in §4.2. For JSON and SMILES, correctness is evaluated by comparing to a golden solution.

Table 2: Constrained decoding (Con. –) consistently increases the percentage of syntactically correct
completions for DLMs over standard decoding (Van.).

		C++			JSON			SMILES		
	Model	Van.	Con.	Con.	Van.	Con.	Con.	Van.	Con.	Con.
Syntax	DREAM 7B DREAMC. 7B LLADA 8B DIFFUC. 7B	40.5 11.0 13.3 39.2	58.7 19.0 36.1 54.7	99.4 99.2 99.7 99.7	22.4 73.7 77.5 64.5	86.6 89.0	100.0 100.0 100.0 100.0	67.5 73.1 58.2 69.3	93.7 94.9 91.3 92.2	99.4 100.0 100.0 99.2
Funct.	DREAM 7B DREAMC. 7B LLADA 8B DIFFUC. 7B	6.6 3.7 3.8 12.5	8.8 4.9 5.0 13.7	9.5 5.2 5.3 14.8	7.4 44.6 43.1 34.3	49.5	14.3 46.7 49.5 38.2	0.6 3.4 0.7 1.1	1.1 3.4 1.0 1.1	1.1 3.4 1.0 1.1

Syntax errors We observe that our method consistently increases syntactic correctness for all tasks and models, as shown in Table 2. Without sampling valid completions (Con. $^-$), our method increases the percentage of syntactically correct instances by 16.1%, 14.7%, and 26.0% for C++, JSON, and SMILES respectively. We observe that many models fail to generate syntactically correct output even under constraints, with, for example, only 19.0% correct C++ generations for DREAM-CODER 7B. However, sampling valid completions (Con.) recovers the failed instances, increasing to 99.2%. In JSON, constrained decoding with completion achieves 100% syntactic correctness.

Functional correctness As shown in the lower half of Table 2, the positive effect of constraining on functional correctness is also present for DLM, with an average increase in functional correctness without completions (Con. $^-$) of 1.9%, and a slight additional boost with completions (Con.) to 2.2%. Notably, DREAM 7B performance on JSON increases by 6.9%. In the SMILES setting, where models perform very poorly at only 1.5% average correctness, syntactic constraints are not able to improve functional correctness significantly, achieving only a modest average increase of 0.2%.

Runtime overhead We compare the runtime to complete samples in constrained decoding with the vanilla setting. The median completion overhead is only 30%. We observe both speed-ups of up to 19% and slowdowns of up to 190%. Speed-ups occur when the decoding is preemptively aborted.

5 Related Work

Large language models LLMs have recently gained traction for diverse tasks such as code generation [23] and structured output generation [2, 27, 41]. While the most common approach trains LLMs for PRE generation, many modern code models also support FIM settings [19, 29, 56]. More recently, diffusion language models have been scaled to billion parameter sizes and demonstrate promising performance on a variety of tasks [17, 36, 54]. Like many recent models, these diffusion models are instruction fine-tuned, enabling them to follow complex natural language instructions [32]. Such models are typically trained on datasets containing billions to trillions of tokens and have billions of parameters, with both factors contributing to improved performance on benchmarks [19, 33, 45, 49]. Meanwhile, LLMs are known to make mistakes during generation. For example, in niche programming languages [15], and even fundamentally struggle to accurately model specific types of formal languages [11, 46].

Leveraging language intersections Two similar works leverage the intersection of CFLs and regular languages. First, Fazekas et al. [12] discuss subsequence matching, which asks whether w is a subsequence of any word in language L. This is a special case of our decision problem, with $\mathbf{x} = \varepsilon \square w_1 \square \ldots \square w_{|w|} \square \varepsilon$, and can also be solved by using the emptiness check for intersection languages. Their work is not applicable to our setting, as it only handles this special case, does not consider practical performance, and does not consider the handling of lexing.

Second, Nederhof and Satta [35] use intersections of weighted CFGs and DFAs for parsing natural language words, using the intersection language as a succinct representation of admissible parses of

lexeme sequences. To reduce the size of these intersections, they also filter non-generating symbols during the intersection construction.

6 Conclusion

We presented the first constrained decoding method for diffusion models, able to handle context-free languages such as C++ and JSON. We showed how to reduce the problem of valid completion to an infilling decision problem solvable using formal language techniques. Our optimized algorithm demonstrates consistent and significant increase in syntactic and functional correctness on a variety of benchmarks and models, while still ensuring efficiency at inference time

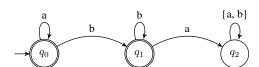
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(a) A DFA where q_0 is the start state, $\{q_0, q_1, q_2\}$ are the states, and q_0 and q_1 are the accepting states. The arrows represent the transition function δ .

$V = \{S, B\}$	(Nonterminals)
$\Sigma = \{a,b\}$	(Terminals)
$S \to aS \mid bB$	΄ ε
$B \to bB \varepsilon$	

(b) A CFG with start symbol S, terminal alphabet $\Sigma = \{a, b\}$, and nonterminals $V = \{S, B\}$. The production rules are the last two lines.

Figure 3: Two representations of a formal language: a DFA (Figure 3a) and a CFG (Figure 3b). Both accept strings that start with a's and end with b's.

A Extended Background on Formal Languages

Formal languages allow to unambiguously specify valid or invalid strings, usually for ensuring machine-readability, i.e., in the case of JSON schemas, or when specifying the syntactic rules of programming languages. Formal languages are, in their most general form, defined as a set of strings over an alphabet Σ . For instance, over the alphabet $\Sigma = \{a,b\}$, one can define the formal language $\{\varepsilon,b,aa,bb,aabb,aaabb,...\}$ of strings consisting of any number of a's followed by b's. In this section, we provide a short explanation of two key classes of formal languages: regular and context-free languages.

A.1 Regular Languages

Regular languages are commonly encountered when describing string patterns with regular expressions. For example, the language of a's followed by b's is described by the regular expression a*b*, where the star denotes zero or more repetitions. A regular language can alternatively be described through a Deterministic Finite Automaton (DFA) that accepts the language [20]. A DFA is a state machine that processes an input string symbol by symbol, transitioning between states based on a deterministic transition function. Thus, a string gets processed by the DFA by starting in the initial state and following the transitions associated with the current input symbol until the end of the string is reached. A string is accepted if the DFA ends in an accepting state after processing the entire string. Formally, a DFA is defined as a tuple $(Q, \Sigma, \delta, q_0, F)$, where: (1) Q is the finite set of states, (2) Σ is the finite alphabet of symbols, (3) $\delta: Q \times \Sigma \to Q$ is the transition function that maps a state and an input symbol to the next state, (4) $q_0 \in Q$ is the initial state, and (5) $F \subseteq Q$ is the set of accepting states. Figure 3a depicts the DFA recognizing the previously introduced language of strings with arbitrarily many a's followed by b's.

In DFAs, the next transition is uniquely determined for each combination of state and input symbol. In contrast, nondeterministic finite automata (NFAs) allow multiple transitions for a state and input symbol combination, making it nondeterministic. One often additionally adds the option to transition between states without consuming any input symbols, through so-called ε -transitions. This added flexibility allows for a more concise depiction and simplifies construction, which is why we use them throughout this work. NFAs accept a word if *any* possible transition according to the input symbols leads to an accepting state. Every NFA (including ε -transitions) can be converted to an equivalent DFA using a standard algorithm [20]. While the minimal DFA constructed for a given NFA may have exponentially many states, the NFAs we construct for the partial LLM outputs can usually be converted into a DFA of around the same number of states.

A.2 Context Free Languages

Context-Free Languages (CFLs) extend regular languages by enabling the expression of recursively nested structures, such as balanced parentheses or properly nested control statements in code. They are described using Context-Free Grammars (CFGs), which consist of production rules that specify how strings in the language can be generated [20]. For most programming languages, the syntactic rules of the language can be adequately captured by a CFG.

CFGs operate with two types of symbols: terminals, which are the actual characters of the language, and nonterminals, which are used to define the language patterns. A CFG is a formal grammar that consists of a finite set of production rules that describe how strings in the language can be generated.

Formally, a CFG is a tuple (V, Σ, P, S) , where: (1) V is a finite set of nonterminal symbols, (2) Σ is a finite set of terminal symbols (with $V \cap \Sigma = \varnothing$), (3) P is a set of production rules of the form $A \to \alpha$, with $A \in V$ and $\alpha \in (V \cup \Sigma)^*$, and (4) $S \in V$ is the start symbol. To generate a string, one starts with S and applies rules from P until the resulting string contains only terminal symbols. This process defines all valid strings in the language. Figure 3b shows a CFG that generates strings over $\{a,b\}$ starting with arbitrarily many a's followed by b's, demonstrating that the same language recognized by a DFA can also be described by a CFG. To generate the string aabb, one could apply the following sequence of production rules: $S \to aS \to aabB \to aabbB \to aabbB \to aabb$.

CFGs are often specified in normal forms, which restrict the grammar to certain types of production rules. The benefit of the resulting language is that it reduces edge cases to handle in productions and simplifies proofs about properties of the language. The most common normal form is the Chomsky normal form, where each production rule is of the form $A \to BC$ or $A \to a$, with $A, B, C \in V$ and $a \in \Sigma$. Many other normal forms exist, such as C2F, which is based on the Chomsky normal form but additionally allows so-called unit production rules of the form $A \to B$ [28]. Languages in Chomsky normal form and C2F can not produce the empty word, as they lack productions that generate the empty string ε [20]. We therefore introduce C2F^{+ ε}, which additionally allows production rules of the form $A \to \varepsilon$.

B Details on Efficient Intersection Language Searches

In this section, we first detail generic optimizations to reduce the size of context-free grammars, then provide a detailed proof of the correctness of our intersection language construction, and finally provide some more details on the search algorithm we employ to decide emptiness.

B.1 Grammar Size Optimizations

The size of the grammar used for the intersection generation is of high importance to the overall runtime, as the number of productions in the intersection grammar scales cubically with the number of productions in the original grammar. While the size of the intersection grammar also depends on the size of the intersected DFA, generic methods to minimize DFAs exist, whereas no such methods are known for CFGs [20].

We therefore apply several heuristics to reduce the grammar size:

- Inlinable terminal elimination: Inline the productions of nonterminals that are only used in a single production. In particular, when B is only used in a single production $A \to \alpha B \beta$, with $B \to \gamma$, remove B and its production and inline it into the production of A to create $A \to \alpha \gamma \beta$.
- Shared 2-gram elimination: For the most frequent BC such that there are several rules of the form $A \to \alpha BC\beta$, (with α, β non-empty) introduce $A' \to BC$ and rewrite $A \to \alpha A'\beta$. Repeat until no more such BC with more than one occurrence can be found.
- Left factoring: We eliminate shared prefixes using left factoring [1]. Specifically, if two productions of the same nonterminal $A \to \alpha\beta$ and $A \to \alpha\beta'$ share the prefix α , we can introduce a new symbol A' and replace the productions to eliminate the duplication, concretely introducing $A \to \alpha A'$ and $A' \to \beta$, $A' \to \beta'$.

After applying these heuristics, we convert the resulting CFG to $C2F^{+\varepsilon}$ using a standard algorithm, consisting of several transformation steps, such as terminal elimination and binarization [28]. In between each step, we detect and eliminate potentially constructed non-generating symbols.

B.2 Construction of the Intersection Language for CFGs in C2F $^{+\varepsilon}$

Since the proof is rarely written out in the literature, highly useful to follow our algorithm, and adapted by us to allow grammars in $C2F^{+\varepsilon}$, we now provide the full constructive proof that the intersection of a CFL and a regular language is a CFL.

Lemma 1. The intersection language $L \cap R$ between a context-free language L and the regular language R is context-free.

Proof. We give a constructive proof by explicitly building a CFG that generates $L \cap R$. We provide the details omitted in the proof given by Gasarch [14] and extend it to allow grammars in C2F^{+ ε}.

Let L_{CFL} be generated by a CFG $G=(V,\Sigma,P,S)$, and let L_R be accepted by a DFA (Q,Σ,δ,q_0,F) . We first convert G to $\text{C2F}^{+\varepsilon}$. Then, we construct a new CFG G_{\cap} whose language is exactly $L_{\cap}=L_{\text{CFL}}\cap L_R$.

The idea is to simulate the CFG G and DFA $(Q, \Sigma, \delta, q_0, F)$ in parallel. Specifically, we define the nonterminals of G_\cap to be of the form ${}^p\vec{A}^q$, where $A \in V$ is a nonterminal of G, and $p, q \in Q$ are states of the DFA. We then create production rules in such a way that if there exists a sequence of productions such that ${}^p\vec{A}^q \to \cdots \to w$, then there exists a sequence of productions in G such that $A \to \cdots \to w$ and G takes the DFA from state G to state G. We then add a start symbol G and productions $G \to {}^{q_0}\vec{S}^f$ for all $G \to {}^{q_0}\vec{S}^f$ for all that also take the DFA from the start state $G \to {}^{q_0}\vec{S}^f$ for an accepting state $G \to {}^{q_0}\vec{S}^f$ for all $G \to {}^{q_0}\vec{S}^f$ for all that also take the DFA from the start state $G \to {}^{q_0}\vec{S}^f$ for all $G \to {}^{q_0}\vec{S}^f$ for all $G \to {}^{q_0}\vec{S}^f$ for all that also take the DFA from the start state $G \to {}^{q_0}\vec{S}^f$ for all $G \to {}^{q_0}\vec{S}^f$ from the start state $G \to {}^{q_0}\vec{S}^f$ for all $G \to {}^{q_0}\vec{S}^f$ for all that also take the DFA from the start state $G \to {}^{q_0}\vec{S}^f$ for all $G \to$

The productions of G_{\cap} are defined as follows (adapting [14], additional rules in green):

- 1. For each production $A \to \sigma$, for all $p, q \in Q$ where $\delta(p, \sigma) = q$, we add $\vec{A} \to \sigma$
- 2. For each production $A \to \varepsilon$, for all $p \in Q$, add $\vec{A}^p \to \varepsilon$
- 3. For each production $A \to BC$, and for all $p,q,r \in Q$, we add $\vec{P}\vec{A}^r \to \vec{P}\vec{B}^{qq}\vec{C}^r$
- 4. For each production $A \to B$, for all $p,q \in Q$, add ${}^p\vec{A} \overset{q}{\to} {}^p\vec{B} \overset{q}{\to}$

The intuition behind the additional rules is that if the automaton is in some state q, we can "switch the current symbol" $(A \to B)$ or "produce an empty string" $(A \to \varepsilon)$ without affecting the state. These productions cover the two additional allowed productions in $C2F^{+\varepsilon}$ grammars, which are not present in CNF grammars.

Finally, we add a new start symbol S' with productions $S' \to {}^{q_0} \vec{S}^f$ for all $f \in F$.

We show that the language generated by the constructed CFG L_{\cap} is equivalent to the intersection language of the CFL L_{CFL} and regular language L_R , i.e., $L_{\cap} = L_{\text{CFL}} \cap L_R$. To do so, we first need some additional notations:

- For any $p,q\in Q$ and $A\in V$, $L({}^p\vec{A}^q)$ denotes the language generated by the nonterminal ${}^p\vec{A}^q$ in the constructed CFG, i.e., the set of all words that can be derived with ${}^p\vec{A}^q$ as the start symbol. Note that $L_{\cap}=\bigcup_{f\in F}L({}^{q_0}\vec{S}^f)$.
- For any $A \in V$, L(A) denotes the language generated by the nonterminal A in the original CFG, i.e., the set of all words that can be derived with A as the start symbol. Note that $L_{\text{CFL}} = L(S)$.
- For any $p,q\in Q$, $L(p\to q)$ denotes the language accepted by the DFA with start state p and final state q, i.e., the set of all words that can be accepted by the DFA starting in state p and ending in state q. Note that $L_R=\bigcup_{f\in F}L(q_0\to f)$.

We will show that for any $p, q \in Q$ and $A \in V$

$$L({}^{p}\overrightarrow{A}^{q}) = L(A) \cap L(p \to q).$$

This immediately implies that $L_{\cap} = L_{\text{CFL}} \cap L_R$, as

$$L_{\cap} = \bigcup_{f \in F} L(^{q_0} \vec{S}^{\ f}) = \bigcup_{f \in F} (L(S) \cap L(q_0 \to f)) = L(S) \cap \bigcup_{f \in F} L(q_0 \to f) = L_{\mathrm{CFL}} \cap L_R.$$

We prove both inclusions separately.

(\subseteq) We show that for any $p,q\in Q$ and $A\in V$, $L({}^p\vec{A}^q)\subseteq L(A)\cap L(p\to q)$. Let the generation path of $w\in L({}^p\vec{A}^q)$ be defined as the sequence of productions that were used to derive w from ${}^p\vec{A}^q$. Denote

 $L_n(\vec{A}^q) = \{w \in L(\vec{A}^q) \mid \text{the generation path of } w \text{ has length } \text{ at most } n\}.$

We show the inclusion by induction over the length of the generation path.

- $\mathbf{n}=\mathbf{1}.$ We show that $L_1({}^p\vec{A}^{\;q})\subseteq L(A)\cap L(p\to q).$ Since w is a word, the only possible productions that can be used to derive w from ${}^p\vec{A}^{\;q}$ are either rule 1 or rule 2. In the first case, we know $w=\sigma, A\to\sigma$ is a production of the original CFG G, and $\delta(p,\sigma)=q$. Hence, $w\in L(A)$ and $w\in L(p\to q)$. In the second case, we have $w=\varepsilon, A\to\varepsilon$ is a production of G, and p=q. Hence, $w\in L(A)$ and $w\in L(p\to q)$.
- n > 1. Suppose that for all $p,q \in Q$ and $A \in V$, $L_{n-1}({}^p\vec{A}^{\;q}) \subseteq L(A) \cap L(p \to q)$. Let $w \in L_n({}^p\vec{A}^{\;q})$ be a word with a generation path of length n > 1. Then the first production rule applied to w cannot be rules 1 and 2, as these would yield a generation path of length one. Hence, the first rule applied must be either of the rules 3 and 4. In the former case, we know there exist two words $w_1 \in L_{n-1}({}^p\vec{B}^{\;r}), w_2 \in L_{n-1}({}^r\vec{C}^{\;q})$ such that $w = w_1 \circ w_2$. By induction, we have $w_1 \in L(B) \cap L(p \to r)$ and $w_2 \in L(C) \cap L(r \to q)$. Since $A \to BC$ is a production of G, we have $w \in L(A)$ as well. Furthermore, since w_1 transitions the DFA from p to r and w_2 transitions from r to q, we have $w \in L(p \to q)$. Hence, $w \in L(A) \cap L(p \to q)$.

 In the latter case, we have $w \in L_{n-1}({}^p\vec{B}^{\;q})$ for some nonterminal $B \in V$ such that $A \to B$ is a production of G. By the induction hypothesis, we have $w \in L(B) \cap L(p \to q)$. Since $A \to B$ is a production of G, we have $w \in L(A)$ as well. Hence, $w \in L(A) \cap L(p \to q)$.
- (\supseteq) We show that $L({}^p\vec{A}^{\;q})\supseteq L(A)\cap L(p\to q)$. Let the generation path of w now be measured with respect to the original CFG, i.e., the sequence of productions that were used to derive w from A. Denote

 $L_n(A) = \{ w \in L(A) \mid \text{the generation path of } w \text{ has length at most } n \}.$

We once again show the inclusion by induction over the length of the generation path.

 $\mathbf{n}=\mathbf{1}.$ We show that for any $p,q\in Q$ and $A\in V$, $L_1(A)\cap L(p\to q)\subseteq L({}^p\vec{A}^q)$. Since w is a word, the only possible productions that can be used to derive w from A directly are $A\to\sigma$ or $A\to\varepsilon$.

In the former case, we have $w=\sigma$, and since a DFA only consumes symbols one-by-one, there must be a corresponding state transition, i.e., $\delta(p,\sigma)=q$. Hence, $w\in L(^p\vec{A}^q)$ by rule 1.

- In the latter case, $w=\varepsilon$, which immediately implies that p=q since a DFA does not contain epsilon transitions. Hence, $w\in L({}^p\vec{A}^q)$ by rule 2.
- $\mathbf{n} > \mathbf{1}$. Suppose that for all $p, q \in Q$ and $A \in V$, $L_{n-1}(A) \cap L(p \to q) \subseteq L({}^p\vec{A}^q)$. Let $w \in L_n(A) \cap L(p \to q)$ be a word with a generation path of length n > 1. Then the first rule applied cannot be $A \to \sigma$ or $A \to \varepsilon$, as these would yield a generation path of length one. Hence, the first rule applied must be either $A \to BC$ or $A \to B$ for some nonterminals $B, C \in V$.

In the former case, we know there exist two words $w_1 \in L_{n-1}(B), w_2 \in L_{n-1}(C)$ such that $w = w_1 \circ w_2$ such that $A \to BC$ is a production in the original CFG. Since $w \in L(p \to q)$, we also know that consuming w transitions the DFA from state p to q. We also know that, starting in q, after consuming w_1 , the DFA will arrive at some intermediate state r. Clearly therefore $w_1 \in L(p \to r)$. Moreover, since $w = w_1 \circ w_2$ and $w \in L(p \to q)$, also $w_2 \in L(r \to q)$. By induction, we then have $w_1 \in L_{n-1}(B) \cap L(p \to r) \subseteq L({}^p\vec{B}^r)$ and similarly $w_2 \in L({}^r\vec{C}^q)$. We know that production ${}^p\vec{A}^q \to {}^p\vec{B}^r$ is in the intersection language, due to rule 3 quantifying over all states in Q. Hence, $w \in L({}^p\vec{A}^q)$.

In the latter case, we have $w \in L_{n-1}(B)$ and $w \in L(p \to q)$. By the induction hypothesis, we have $w \in L({}^p\vec{B}^q)$. Since $A \to B$ is a production of the original CFG, we have $w \in L({}^p\vec{A}^q)$ as well by rule 4.

This completes the proof of the lemma.

B.3 Details on the Search Algorithm

We explain in detail how the search algorithm for generating nonterminals in the intersection language works. The corresponding pseudo-code is presented in Algorithm 2. We leverage the construction rules of the intersection language to conduct the search on the *implicit* intersection grammar, i.e., we only build the parts of the grammar that we need to explore. Nonterminals in the intersection language have the form \vec{A}^q for $p,q \in \Sigma$ and $A \in V$. All production rules of the form $\vec{A}^q \to \varepsilon$ and $\vec{A}^q \to \sigma$ are based on the corresponding productions $A \to \sigma$ (Construction 1) and $A \to \varepsilon$ (Construction 2) in the original grammar. We leverage this insight to perform the initialization of the search, which iterates over all production rules of this format, at the beginning of the algorithm in Lines 2–5. Further, all other productions are of the form $\vec{A}^q \to \vec{B}^q \vec{C}^r$ and $\vec{A}^q \to \vec{B}^q \vec{C}^q$, as constructed by Constructions 3 and 4. Importantly, all rules for all combinations of states p,q,r exist. This allows us to enumerate all such rules for a given symbol B or C on the fly, as done in Lines 9–17, without expending unnecessary execution time. For example, in Line 9, we iterate over all production rules in which the nonterminal \vec{X}^z occurs. The two states of the DFAs already fixate two of the three states quantified over in Construction 3. Hence, given a production $A \to XC$ in the original grammar, which uses the nonterminal X and additional nonterminal X0 we need to iterate over a single additional state variable X1 to evaluate all corresponding constructed productions $\vec{X}^q \to \vec{X}^q \times \vec{$

C Lexing with LLM Tokens

Discrepancies between alphabet and LLM tokens The approach described in §3.2 operates directly on the formal language alphabet Σ . For practical purposes, this alphabet usually consists of *lexemes* which are extracted from a character-level string into a shorter and more abstract representation in a process called *lexing*. For programming languages, these lexemes could be identifiers, literals, operators, and other syntactic elements of the language, such as if and else. The code generation paradigms addressed in this work generate code on a character level and thus require lexing before we can apply our method. In addition to the normal lexing process, our approach needs to handle the partial nature of the LLM outputs, taking into account potential partial lexemes and consequently several possible lexing sequences for the same character-level output. In the remainder of this section, we first explain how to convert the partial LLM output to a set of possible lexeme sequences, and then how to apply the constrained infilling algorithm to these lexeme sequences.

Lexemes and lexing Each lexeme is described via a regular language with Σ being the set of Unicode characters. For example, the <number> lexeme is described by regular expression \d+, and the <identifier> lexeme by [a-zA-Z_]\w*. Lexing is the process of converting a character-level string into a sequence of lexemes, i.e., a sequence of strings that match the regular expressions of the lexemes. We call such a sequence of lexemes a *lexeme sequence*. The algorithm extracts these sequences by iteratively matching the maximum match for all lexemes that match a nonempty string at the beginning of the currently remaining output. Most commonly, whitespaces between lexemes are stripped. For example, the character-level string "1234 hello12" would be lexed into the lexeme sequence (<number>,<identifier>).

Lexing partial outputs For a partial output x with infilling regions, we extract the represented lexeme sequences for each chunk of continuous text. For instance, the output "x = 1234 | hello12" would be split into the chunks "x = 1234" and "hello12", which would be lexed into the two lexeme sequences (<identifier>, <=>, <number>) and (<identifier>). Note that the resulting list

of lexeme sequences is a list of words in Σ that can be directly used to construct the regular language for the infilling problem as described in §3.2, for example here forming the infilling problem "<identifier>"=><number> \square <identifier>".

Handling lexemes spanning infilling regions However, the lexing process is not as straightforward as described above because lexemes can span over the infilling regions in the output. For example the output "pl23" could be lexed as (<number>). However, the region could be filled with token "a", resulting in the overall lexing (<identifier>). To correctly handle these cases, we must also take into account the suffixes and prefixes of lexemes when adjacent to an infilling region.

Additionally, lexemes may span over an entire infilling region. For example, for the output "123 \square 789", the lexing would yield the lexeme sequences (<number>) and (<number>). However, it is also possible to insert a token "456" into the region, such that the lexing of the final character-level text is just a single lexeme sequence (<number>). In particular, for any chunk $\alpha\beta$ ending with a prefix β of a lexeme a and a consecutive chunk $\gamma\eta$ starting with a suffix γ of the same lexeme <a>, then a valid corresponding lexeme sequence for the entire chunk sequence would be $(lex(\alpha), <a>, lex(\eta))$.

Note that we need to additionally ensure the prefix and suffix of the lexeme are compatible. For instance, for fixed-width lexemes such as <while>, we can not insert a token into the sequence "whipile" to obtain a sequence with only a single lexeme, even though both "whi" and "ile" are true prefixes and suffixes of the lexeme while. We resolve this by storing the exact partially matched parts of the lexeme and deciding the infilling problem with respect to the lexeme's regular language. This effectively generalizes a similar solution to the one proposed by Melcer et al. [31], in which they explicitly store the reached states within each prefix and suffix and ensure reachability between them.

Lexing algorithm We use some helper operations on character-level DFAs for the lexing algorithm. For DFA D, we define the function MATCH, which returns l, the number of characters in the string that the suffix language automaton matches maximally. For example, \d +.MATCH(123) = 3 and \d +.MATCH(1hello) = 1. The function \d PREFIX(D) returns the true prefix language of D, where a *true* prefix is a prefix that can be completed to a full match by appending at least one more character. For example, 123 is a true prefix for \d + but not for \d 0. 12 is a true prefix for both regular expressions. The function \d UFFIX(D) analogously returns the true suffix language of D. Further, we denote as \d =1 the string formed by first \d 1 characters of \d 2 and \d 3 and \d 5 the string formed by all characters after the first \d 3 characters in \d 6.

The lexing algorithm applied to each chunk of continuous text in \mathbf{x} is described in Algorithm 3. The main mode of operation is to keep track in S of possible lexings and remainders to be processed, starting with the empty lexing and the entire string to be processed in Line 1. The method then iterates over all these lexings in Line 8, returns them if the remainder is empty (Line 10) or extends them if a non-empty remainder remains (Line 11). Crucially, Lines 2–7 check whether the text starts with the suffix of any lexeme. This is relevant for generations with infilling, as opposed to prefix constraining, where only prefixes at the end are possible. Additionally, Line 12 checks whether the remainder of the current text is the prefix to some lexeme.

Applying the constrained infilling algorithm Applying the lexing algorithm to every continuous chunk of text in the partial output results in a list of sets of lexeme sequences, or sets of words in our infilling problem. From this list, we obtain a set of lists of words by taking the cross product of all the sets in the list, e.g., for list $(\{(\alpha, \beta)\}, \{(\gamma), (\eta)\})$, we would obtain the two lexeme-level partial outputs $\alpha\beta\Box\gamma$ and $\alpha\beta\Box\eta$.

If we decide for any of the resulting lexeme-level partial outputs that the intersection language L_{\cap} is non-empty, then the current character-level partial output is valid, and we can continue generation. If no lexeme sequence results in a non-empty intersection, then we need to reject the current output. Thus, we have to apply the infilling algorithm to each of the word lists derived from the lexing process. In practice, we may derive a large number of lexeme sequences, as different possibilities from text chunks get combined and result in a combinatorial explosion. To further optimize the lexing process, we add two additional optimizations, which we describe in the following paragraphs.

Algorithm 2 Deciding intersection emptiness of a CFG and DFA. The CFG is in CNF. G.ADD(x) inserts x into G and returns true if x was not in G previously.

```
Input: CFG C, DFA R = (Q, \Sigma, \delta, q_0, F)
Output: L(C) \cap L(R) = \emptyset
       1 G \leftarrow \emptyset
                   for all productions A \to \sigma do
                                                                                                                                                                                                                                                                                       ▶ Mark terminal and epsilon productions.
                                G \leftarrow G \cup \{ {}^{p}\vec{A}^{q} | \delta(p, \sigma) = q \}
                    for all productions A \to \varepsilon do
                                G \leftarrow G \cup \{ {}^{p}\vec{A}^{p} | p \in Q \}
                   s \leftarrow G.COPY()
                     while s \neq \varnothing do

    ▷ Explore all remaining productions

                                {}^{y}\vec{X}^{z} \leftarrow s.POP()
                                for all productions A \to XC, all q \in Q do
                                          if \vec{C}^q \in G and G.ADD(\vec{A}^q) then
   10
                                                        s.add(\vec{A}^q)
   11
                                for all productions A \to BX, all q \in Q do
   12
                                           if {}^{q}\vec{B}^{\ y} \in G and G.ADD({}^{q}\vec{A}^{\ z}) then
   13
                                                         s.ADD(\overset{q}{\vec{A}}^z)
   14
                                for all productions A \to X do
   15
                                           if G.ADD(^{y}\vec{A}^{z}) then
   16
                                                        s.ADD(\vec{A}^z)
   17
              \mathbf{return} \ G \cap \{ \stackrel{q_0}{\vec{S}} \stackrel{f}{\mid} f \in F \} = \varnothing \qquad \triangleright \text{ Whether any start symbol of } L(C) \cap L(R) \text{ is generating } P(C) \cap P(R) \text{ is generating } P(C) \cap P(C) \text{ is generating } P(C
```

Algorithm 3 Extracting lexings of partial output

```
Input: Input string w, Terminals T
Output: Set \{(x_i, s_i, p_i)\}_{0 \le i \le n} of n possible lexeme sequences x_i and optional partial matches to
     the first (s_i) or last (p_i) lexeme
 1 S \leftarrow \{(\varepsilon, w, \text{None}, \text{None})\}
     for t \in T do
                                                 Determine if the string starts with a suffix of any terminal
         if SUFFIX(PREFIX(t)).MATCH(w) = |w| then \triangleright If the suffix prefix spans the entire word.
              S.ADD(t, \varepsilon, w, w)
 4
         l \leftarrow \text{SUFFIX}(t).\text{MATCH}(w)
 5
         if l > 0 then
                                                                  \triangleright If the suffix matches a non-zero prefix of w
              S.ADD(t, w_{>l}, w_{< l}, None)
     while S \neq \emptyset do
         (x, w, s, p) \leftarrow S.POP()
         if w = \varepsilon then yield (x, s, p)
10
         for t \in T do
11
              if PREFIX(t).MATCH(w) = |w| then
                                                               ▶ If the prefix spans the entire remaining word.
12
                   S.ADD(x \circ t, \varepsilon, s, w)
13
              l \leftarrow t.\text{MATCH}(w)
14
              if l > 0 then
                                                                  \triangleright If the suffix matches a non-zero prefix of w
15
                   S.ADD(x \circ t, w_{>l}, s, None)
16
```

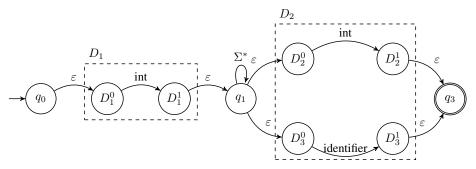


Figure 4: A union automaton in the second half of the DFA for output "123 $\ \square$ 789", accounts for the possibility to lex the second half as either <int> or <identifier>. The resulting automaton accepts both valid lexeme sequences <int><int> and <int><identifier>.

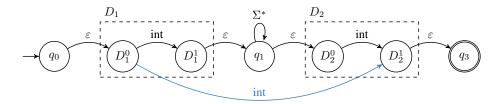


Figure 5: A skip connection, highlighted in blue, in the DFA for output "123 $\,\Box$ 789", accounts for the possibility to lex the input as a single <int>. The resulting automaton accepts both valid lexeme sequences for a single int and two ints with intermediate tokens. This construction can be combined with Figure 4.

Optimizing subset lexemes We avoid a combinatorial explosion of possible lexeme sequences by automatically removing lexemes where the accepted language is a subset of the accepted language of another lexeme. For example, in SMILES, the string "5" could be interpreted as <digit> or as <fifteen>, which is a special lexeme only allowing numbers from 1 to 15. We resolve this by automatically detecting lexemes α that accept a subset of valid strings of another lexeme β , and a) remove the subset α from the accepted language of lexeme β , and b) allow the lexeme α at any position in the grammar where either the subset token or the full token is allowed, in particular we substitute terminal β with $\alpha \mid \beta$. This optimization reduces the number of extracted sets of possible lexeme sequences for each continuous chunk of text.

We further manually reduce the number of lexemes that overlap and lexemes that are prefixes or suffixes of other lexemes, such as <++> and <+>, to further optimize performance.

Combining lexeme sequences to single NFA To avoid explicitly enumerating all possible combinations of lexeme sequences of a string, we directly derive a single, larger NFA that accepts all possible combinations of lexeme sequences at the same time. This union of NFAs is structurally similar to the NFAs of each lexeme sequence, but adds alternative paths for mergeable lexemes. While this NFA grows linearly in the number of sequences, these merges result in a smaller NFA than the union of all lexeme sequences and thus improve performance.

If a text chunk has two or more admissible lexings, we can replace the constructed D_i with the union NFA. For example, the output "123 \Box 789" must also admit recognizing the second chunk as the suffix of an identifier. Thus, we obtain the two sequence sets $\{(<int>)\}$ and $\{(<int>)\}$, $(<identifier>)\}$. By generating a single NFA that accepts both sequences (<int>) and (<identifier>), we can construct a single NFA by applying the concatenation construction to the standard NFA for the first lexeme sequence and the unionized NFA for the second sequence. The resulting NFA is presented in Figure 4.

Another example is depicted in Figure 5. Here, for the previously shown output "123 \square 789", the first chunk ends with a prefix of the lexeme <int>, and the second chunk starts with a suffix of the same lexeme. In addition to the standard construction for the possible extracted list (<int>, <int>),

we add an <int>-edge from the second-to-last state of D_0 to the second state of D_1 , resulting in an alternative path that accepts the list (<int>). These paths are constructed by maintaining a list of suffixes of previous D_i when constructing D_{i+1} , and adding the edge in case that a suffix matches a prefix of the lexing of D_{i+1} .

These constructions allow avoiding the combinatorial explosion that necessarily arises from ambiguous lexings of the same partial output.

D Experimental Details, Ablations and Case Study

In this section, we provide additional details about the implementation, hyperparameters, datasets, runtime overhead, an ablation on the number of diffusion steps, and a case study.

D.1 Implementation

Overview Our implementation is written in around 7000 lines of Python and 5500 lines of Rust. The main logic, concerning LLM sampling and CFG and DFA construction, is written in Python, with the more computationally expensive formal language operations, such as Algorithms 2 and 3, implemented in Rust, compiled as Python bindings. Several low-level formal language operation implementations are inspired by the educational Python implementations by Romero [44].

Grammars Our C++ grammar covers a comprehensive but not complete subset of C++, with all features used in the canonical solutions of the translated dataset implemented, but advanced features like template functions and classes not supported. Moreover, we disallow the insertion of multi-line comments inside function bodies, as this allows the model to generate arbitrary and broken code that is syntactically valid as long as it is finally wrapped in the multi-line comment delimiters. We further restrict models in the FIM setting to not generate additional function signatures and bodies to prevent the generation of additional main functions or test cases.

We preprocess all model outputs by marking word boundaries with special \langle and \rangle tokens that do not appear in the original text and are never generated by the model¹. For example, the string int main() is converted to \langle int \rangle \langle main \rangle (). This enables us to check for such word boundaries inside the grammar, i.e., being able to distinguish whether white-space was present between symbols even after it is stripped in the lexing process.

The JSON schema grammars are obtained dynamically based on the JSON Schema for each task. We recursively build up the grammar based on the provided specification. For SMILES, we implement the specification described by Apodaca [3], which is a more precise and efficient variant of prior specifications [43, 52].

D.2 Models and Hyperparameters

All methods were run four times, with seeds 0 to 4, and we report the averaged results in all tables. We report the maximum among Van., Con.⁻, and Con. decoding with **boldface**. We <u>underline</u> all results where the confidence interval of the improvement over the given method is not positive at 95%. We limit the amount of generated tokens to 256 and time out if generation does not complete after 300 seconds.

Sampling algorithms and temperature All MRI models were sampled with temperature 1 and greedy decoding. The diffusion models are sampled with a temperature of 0.2. To pick a token from the diffusion models distribution, we use the entropy algorithm for the DREAM 7B based models, DREAM 7B, DREAMCODER 7B, and DIFFUCODER 7B, and low confidence for the LLADA 8B model, as recommended by the model developers.

Diffusion steps When not explicitly stated otherwise, the diffusion models are run with 32 diffusion steps. Diffusion language models can be run with a varying number of diffusion steps, determining how many tokens are sampled from a single model inference [36, 55]. Lower numbers of steps imply more tokens being sampled from each inferred distribution. One of the key benefits of

¹In particular, we use the bytes \x02 and \x03

diffusion language models is to exploit this ability, resulting in overall faster decoding. At the same time, higher numbers of steps are usually associated with increased accuracy on the requested task, as the model can adapt its distribution to newly inserted tokens. Our choice of step size 32 represents a trade-off between speed and accuracy.

When the number of diffusion steps k is not equal to the number of generated tokens n, the model $\frac{n}{k}$ tokens are sampled from every model diffusion step, which generates a single distribution each. During constrained decoding, we iteratively sample single tokens from this distribution according to the respective algorithms (low confidence or entropy), masking out and resampling after a rejection. When a token is accepted, we mask out the token's index from the distribution. We then run model inference again after $\frac{n}{k}$ tokens have been accepted.

D.3 Datasets

C++ We leverage the C++ translation of HumanEval in the HumanEval-X dataset [57]. It contains 164 instances of simple programming problems and canonical solutions written by humans. For the MRI tasks, we remove between 1 and 3 randomly sized spans of 5 to 100 characters from these canonical solutions, generating one MRI task per instance in the original dataset. If we end up with insufficient remaining characters after removing the required number of spans, we resample sizes and positions up to 3 times, aborting if we do not find a valid removal. Additionally, we remove 5 human-written solutions that are not valid according to our implementation of the syntax, i.e., because they contain multi-line comments or additional helper functions. This results in three MRI datasets of 159, 156, and 143 samples in 1-MRI, 2-MRI and 3-MRI respectively. An example prompt for an instance from the dataset is presented in Figure 7. For DLM, we use all 164 tasks of the original dataset and extract the comment before the function as an instruction for the model. An example prompt is shown in Figure 8.

We check the functional correctness in both settings by checking whether all test cases in the dataset pass with the model-generated solution.

JSON Schema We extend the JSON-Schema dataset by NousResearch [37]. Concretely, the dataset originally contains a unique schema per task. We clean the schemas by disallowing properties other than specified on the top level and repairing instances that accidentally do not require any fields. We then extend the dataset by sampling GEMINI-2.5-PRO for 10 inputs and completions for each schema. We filter these samples in three ways to ensure high quality.

First, we filter the resulting extracted outputs for syntactic validity according to the schema and discard invalid generations. Second, we require GEMINI-2.5-PRO to be able to solve the task, i.e., the model must generate a valid JSON object that passes the schema validation if it is only given the input and the schema. Third, we perform fuzzy matching to deduplicate the resulting samples. This process results in 272 instances. The prompts used for generation and verification are shown in Figure 11 and Figure 12. An example prompt for this task is shown in Figure 9.

We evaluate functional correctness on this dataset by checking for exact equality between a normalized JSON dump of the golden solution and the model-generated solution.

SMILES To create a benchmark for SMILES, we query GEMINI-2.5-PRO to generate pairs of descriptions of molecules and their SMILES notation. Again, we perform three filtering steps to ensure high quality. First, we verify that the generated molecule is valid using the Rdkit library [26]. Second, we ensure the model can generate the correct SMILES string for the molecule if it is only given the description. Third, we filter out duplicates using fuzzy matching. This results in 167 unique pairs of descriptions and SMILES strings. Prompts for this generation procedure are shown in Figure 13 and Figure 14. An example prompt for this task is shown in Figure 10.

To check functional correctness of the model-generated molecule, we parse it using Rdkit and check the equivalence to the molecule generated by GEMINI-2.5-PRO in canonical representation.

D.4 Additional Experiments

Runtime overhead For all experiments in §4, we measure the runtime of our constraining method and unconstrained decoding. We present a detailed comparison in Tables 3 and 4.

Table 3: Median overhead per token for different infilling settings in ms and percent increase over unconstrained generation. Larger models with higher inference time experience a lower slowdown due to constraining. More infilling regions also increase constraining overhead.

#Regions	1-mri	2-mri	3-mri
CODEGEMMA 7B	3.1 _{↑47%}	$4.1_{\uparrow 63\%}$	6.4 _{\(\frac{1}{2}\)99\%}
STARCODER2 7B	$3.3_{159\%}$	5.5 _{↑98%}	$9.7_{\uparrow 190\%}$
DEEPSEEK C. 1.3B	$3.6_{\uparrow 158\%}$	$5.8_{\uparrow 245\%}$	$11.8_{\uparrow 557\%}$
DEEPSEEK C. 6.7B	$3.0_{158\%}$	$4.6_{\uparrow 90\%}$	$7.7_{\uparrow 153\%}$
DEEPSEEK C. 33B	$3.1_{\uparrow13\%}$	$4.3_{\uparrow19\%}$	$6.5_{\uparrow28\%}$

Table 4: Median time difference per completion for different diffusion models in seconds and the percentual overhead over the original completion. When the completion aborts pre-emptively, as no valid completion is sampled from the model, speed-ups are possible.

Model	C++	JSON	SMILES
Dream 7B	$1.1_{\uparrow 36\%}$	$0.4_{\uparrow 20\%}$	$0.0_{\uparrow 0\%}$
DreamC. 7B	$7.8_{\uparrow 190\%}$	$0.1_{15\%}$	$0.0_{\uparrow1\%}$
LLADA 8B	$-1.0_{\downarrow 19\%}$	$0.5_{\uparrow 9\%}$	$0.0_{\uparrow1\%}$
DIFFUC. 7B	$2.2_{\uparrow 74\%}$	$0.1_{\uparrow 6\%}$	$0.0_{\uparrow2\%}$

In MRI we compare time per token, as constrained decoding often rejects finalizing the current output, thus making completions longer and finalization times incomparable. The median runtime overhead of constrained decoding is 125%, where the overhead on the small DEEPSEEK CODER 1.3B is higher (320%) than on the 7B models (100%) and DEEPSEEK CODER 33B (20%). Moreover, an increasing number of infilling regions also increases the overhead, growing from 67% on 1-MRI to 205% on 3-MRI, as longer prefixes and more infilling regions increase the cost of the intersection algorithm.

For DLM, we compare the total runtime to finish the diffusion decoding process. The average completion overhead is only 30%, but varies strongly between domains. We observe both speed-ups of up to 19%, for LLADA 8B on C++, where many decodings are preemptively aborted, and slow-downs of up to 190%, for DREAMCODER 7B on the same dataset.

Ablation on diffusion steps We evaluate our method on common diffusion step numbers, from 16 to 256, where the lowest setting 16 implies that a single inference step inserts $\frac{256}{16} = 8$ tokens at once, while the highest setting 256 implies that every inference step inserts only a single token.

We present the results of this ablation on DREAM 7B in Table 5 and demonstrate that our method consistently improves syntactic correctness in all settings by on average 14%. Functional correctness on JSON also significantly increases by 1.2%, while the increase in C++ is 0.7% and 0.5% in SMILES. Moreover, the runtime overhead, shown in Table 6, decreases with the number of diffusion steps, from 14% - 108% down to 9% or even a speed up of 3%.

D.5 Case Study

For a qualitative evaluation, we manually inspect instances where unconstrained decoding fails and our type constraining approach successfully corrects errors. We showcase three such examples in Table 7.

Preventing use of invalid types In Table 7a, DREAM 7B generates a summary of a financial review for task #30 in our JSON dataset. The schema requires to output three key values as float numbers. Meanwhile, the model attempts generating the values as strings. Due to the derived language for the JSON schema, it can be determined that the strings are misplaced, not constituting one of the required keys and impossible to match the intended value formatting, and all attempts at placing such strings are thus rejected. Instead, the model generates the values without quote wrapping, resulting in a valid and correct result.

Table 5: Percent syntactically and functionally correct generations for DREAM 7B based on varying number of diffusion steps. Our method consistently increases syntactic correctness in all settings, even when model accuracy increases with step sizes.

		C++			JSON			SMILES		
	#Steps	Van.	Con.	Con.	Van.	Con.	Con.	Van.	Con.	Con.
	16	8.1	20.3	99.2	7.3	24.4	100.0	41.1	80.5	99.7
×	32	40.5	58.7	99.4	22.4	44.9	100.0	67.5	93.7	99.4
nta	64	60.1	74.7	99.8	67.4	73.2	100.0	79.2	94.9	100.0
Syntax	128	81.1	90.7	100.0	90.2	94.0	100.0	80.1	95.8	100.0
	256	98.2	98.2	100.0	95.2	98.2	100.0	80.7	93.4	100.0
_	16	1.4	2.7	4.9	1.5	2.3	3.4	0.6	1.1	1.1
ona	32	6.6	8.8	9.5	7.4	11.4	14.3	<u>0.6</u>	1.1	1.1
Sti.	64	21.0	21.8	22.4	41.8	42.1	42.8	2.4	3.0	3.0
Functional	128	24.5	23.9	24.1	50.7	51.5	51.5	3.1	4.0	4.0
Ţ	256	34.1	34.1	34.8	54.8	54.8	54.8	<u>4.9</u>	5.2	5.2

Table 6: Time difference per completion for different step sizes on DREAM 7B diffusion, in seconds, and the percentual overhead over the original completion. For larger numbers of diffusion steps, overhead reduces from 14%-108% down to 9% or even a speedup of 1%.

#Steps	C++	JSON	SMILES
16	$1.7_{\uparrow 107\%}$	$2.1_{\uparrow 108\%}$	$0.0_{\uparrow 14\%}$
32	$1.1_{\uparrow 36\%}$	$0.4_{\uparrow20\%}$	0.0_{-}
64	$0.6_{\uparrow 18\%}$	$0.1_{\uparrow 4\%}$	$-0.2_{\downarrow 3\%}$
128	$0.4_{\uparrow 10\%}$	$0.2_{\uparrow 4\%}$	$-0.4_{\downarrow 3\%}$
256	$0.8_{\uparrow 9\%}$	$-0.1_{\downarrow 1\%}$	$0.2_{\uparrow 1\%}$

Preventing inadequate nesting In Table 7b DREAMCODER 7B generates an invalid SMILES molecule for task #166 by closing more parentheses than it opened. Since the CFG for SMILES correctly handles counting of nesting levels, attempts to generate the closing parenthesis are rejected by our method. Instead, the model decides to end the generation.

Preventing inadequate syntax In Table 7c, DEEPSEEK C. 6.7B uses Python-style parenthesesless conditions in an if-statement when writing a string processing function in task #150 of our C++ dataset. Since this is invalid in C++ syntax, our method can correct this mistake successfully, forcing the model to add parentheses around the condition.

E Discussion

Remaining syntax errors While our method achieves substantial improvements in syntactic correctness, using only Con. $^-$ still leaves a considerable gap until guaranteeing correctness. We attribute most of this gap to the overapproximation of allowing an arbitrary number of tokens to fill regions in the partial output, as done in prior work [6, 50]. In practice, the LLM is typically limited, i.e., in FIM and MRI it can only generate up to the user-defined maximum, and in DLM it can only generate one token per mask \bot . Examples of this issue occurring are presented in Figure 6b, where the DLM model needs to open several molecule branches in a single remaining token, and in Figure 6a for MRI, where the model exceeds the token limit of 256 tokens as it generates large amounts of unnecessary code.

One approach to resolve this issue would be to accurately model the remaining number of tokens in our regular language construction. However, we observe in experiments that this significantly increases the size of the regular language, as it consequently needs to keep track of the number of inserted tokens. This drastically increases the size of the intersection language, rendering our method too expensive for practical application.

```
vector<string> numerical_letter_grade(vector<float> grades){
       vector<string> out={};
       for (int i=0;i<grades.size();i++)</pre>
4
           if (grades[i]>=3.9999) out.push_back("A+");
5
           if (grades[i]>3.7001 and grades[i]<3.9999) out.push_back("A");</pre>
6
           if (grades[i]>3.3001 and grades[i]<=3.7001) out.push_back("A-");</pre>
           if (grades[i]>3.0001 and grades[i]<=3.3001) out.push_back("B+");</pre>
           if (grades[i]>2.7001 and grades[i]<=3.0001) out.push_back("B");</pre>
            if (grades[i]>2.3001 and grades[i]<=2.7001) out.push_back("B-");</pre>
10
            if (grades[i]>2.0001 and grades[i]<=2.3001) out.push_back("C+");</pre>
11
            if (grades[i]>1.7001 and grades[i]<=2.0001) out.push_back("C");
12
            if (grades[i]>1.3001 and grades[i]<=1.7001) out.push_back("C-");</pre>
13
            if (grades[i]>1.0001 and grades[i]<=1.3001) out.push_back("D+");</pre>
14
            if (grades[i]>0.7001 and grades[i]<=1.0001) out.push_back("D");</pre>
15
            if □ i]<=3.0001) out.push_back("B");</pre>
16
           if (grades[i]>2.3001 and grades[i]<=2.7001) out.push_back("B-");</pre>
17
           if (grades[i]>2.0001 and grades[i]<=2.3001) out.push_back("C+");</pre>
18
```

(a) STARCODER2 7B exceeds the token limit in task #81 in 1-MRI.

Vanilla	Constrained ⁻	Constrained
C6CCCC1)	C6CCCC⊥))	C6CCC(c(c)(c))

(b) LLADA 8B leaves a single \perp for completion in task #153 in SMILES.

Figure 6: Syntax errors may remain when the model has fewer tokens left to complete than would be required to fulfil the syntactic constraints. This can happen both in MRI (a), when the model exceeds the maximum number of generated tokens and in DLM (b), when the model has few mask tokens \perp remaining.

Another approach would be to train the model to insert special tokens that signal requiring additional tokens. For FIM this naturally occurs when the model does not generate an end-of-string token. For DLM a special token could be added to shift tokens beyond the current mask token to the right, adding mask tokens into the completion sequence at the specified position. Such an approach was suggested in concurrent work on new diffusion model training approaches, as this appears to generally improve model performance [53].

Our chosen approach to mitigate the issue is to automatically fill in the output based on the requirements in the language (Con.). However, it cannot rely on the model's probability distribution to steer generation. Determining the most effective way to handle this limitations is an important topic for future work.

Leveraging incremental parsing While we take several steps to improve the efficiency of our method, it can still require a significant amount of time to determine the emptiness of the intersection language after each generated token. Future work may leverage the fact that the CFG for the intersection is fixed and the DFA is only updated using small modifications. This may lead to an approach for incrementally computing emptiness checks by reusing the results of the previous intersection computation. Other approaches to leverage the incremental nature of the parsing, similar to the approaches of Melcer et al. [31], Ugare et al. [50], and Mündler et al. [34] would likely also be able to decrease the worst case and practical overhead of the constraining method.

Context-sensitive language features While our method is designed for context-free languages, an interesting future direction would be extensions to handle more powerful language classes, such as context-sensitive languages. Similar to Melcer et al. [31] and Ugare et al. [50], simple context-sensitive syntactic features can likely be handled by preprocessing through adequate lexers. Beyond syntactic features, prior work suggested leveraging more semantic insights, such as type systems

[34], for constructing more powerful constraint systems. Type checkers with typed holes [38] could be leveraged to achieve such systems.

F Prompts

In this section, we detail all prompts used for the respective models and tasks.

MRI Since models used for FIM and MRI tasks are not instruction-fine-tuned, we provide the model with the raw code, including only a comment above the function to guide the model for completions. We use the standard templating suggested for each model to format the prompt for FIM and MRI completion. If MRI is not supported explicitly, we emulate it by inserting <T0D0> into the remaining infilling regions and repeatedly prompting the model for FIM completion on the first infilling region. In order to prevent the models from generating main methods and tests in the MRI setting, we add a main method at the end of the context that is marked with a TODO comment. An example prompt for the 2-MRI setting is provided in Figure 7.

DLM The models used for DLM tasks are instruction-fine-tuned, allowing us to specify the completion intent in natural language. We provide a general description of the task in the system prompt and the specific task content as the first user prompt. The assistant response is prefilled with the start of a code fence and, in the case of C++, with the necessary header declarations and function signature to ensure results can be extracted and tests can be executed correctly. The prompts for C++, JSON and SMILES tasks are presented in Figure 8, 9 and 10 respectively.

Benchmark generation prompts As outlined in Appendix D, we generate the JSON and SMILES dataset synthetically by prompting GEMINI-2.5-PRO. We provide the used prompts for generation and validation of the generated samples in Figures 11–14.

Table 7: Three examples demonstrating the impact of constrained decoding on DLM and MRI completion. Left are unconstrained completions (Van.) with problematic tokens highlighted in red , and right constrained completions (Con.) with corrections highlighted in green , adapted for clarity. In (a) DREAM 7B our method corrects the type of values in a summary of a financial review for task #30 in our JSON dataset. In (b) DREAMCODER 7B our method prevents closing more parentheses than are opened when generating a SMILES molecule for task #166. In (c), DEEPSEEK C. 6.7B our method forces adding parenthesis around a Python-style parentheses-less condition in an if-statement when writing a string processing function in task #150 of our C++ dataset.

```
Vanilla
                                                                      Constrained
      // summarize my financial review
                                                      // summarize my financial review
        "capitalGains": "5210.5000",
                                                        "capitalGains": 5210.5000,
(a)
        "interestIncome": "1340.25",
                                                        "interestIncome": 1340.25,
        "totalReturn": "4.5"
                                                        "totalReturn": 4.5
      // generate an allene with axial chirality
                                                      // generate an allene with axial chirality
(b)
                                                      C1=CC1=CC(C(00)0)C(00)0
      C1=CC1=CC(C(00)0)C(00)0)C(00)0
      // seperate the groups of nested parentheses
                                                      // seperate the groups of nested parentheses
      if (chr=='(')
                                                      if (chr=='(')
          level+=1;
                                                          level+=1;
(c)
          current_paren+=chr;
                                                          current_paren+=chr;
     }
                                                      }
                                                      else if (chr==')')
      else if chr==')'
```

```
1 region 0
       From a given vector of integers, generate a vector of rolling maximum element found
       until given moment in the sequence.
       >>> rolling_max({1, 2, 3, 2, 3, 4, 2})
       {1, 2, 3, 3, 3, 4, 4}
7
      */
       #include<stdio.h>
       #include<vector>
       using namespace std;
10
       vector<int> rolling_max(vector<int> numbers){
11
           vector<int> out;
12
13
14 region 1
           for (int i=0;i<numbers.size</pre>
15
16
17 region 2
18
           return out;
19 }
20
21 int main(){
       // TODO
23 }
```

Figure 7: Example prompt for the 2-MRI task #1. The intial comment and function signature in blue are derived from the dataset prompt, and the remaining code snippets in green are the remainders of the canonical solution with two randomly removed spans. We append a stub main function to prevent the model from attempting to generate a main function of its own.

```
1 system
      You are an expert in C++ programming. Solve the given problem by writing solution
       code in C++.
3
      When answering, insert the solution code in a ```cpp...``` block. Do neither include
4
       test cases not a main function.
5
7 user
      Check if in given vector of numbers, are any two numbers closer to each other than
8
      given threshold.
9
      >>> has_close_elements({1.0, 2.0, 3.0}, 0.5)
11
      false
      >>> has_close_elements({1.0, 2.8, 3.0, 4.0, 5.0, 2.0}, 0.3)
12
13
14
15 assistant
       ```cpp
16
 #include<stdio.h>
17
 #include<vector>
18
 #include<math.h>
 using namespace std;
20
 #include<algorithm>
21
 #include<stdlib.h>
22
 bool has_close_elements(vector<float> numbers, float threshold){
```

Figure 8: Example prompt for the C++ task #1. The system prompt in black is fixed, whereas the user prompt in blue is extracted from the comment preceding the function and the assistant response is prefilled with a codefence, and in green, headers, and the function signature of each task.

```
1
2 system
 You are a helpful assistant that answers in JSON. Here is the JSON schema you must
 adhere to:
4
 <schema>
5
 {
6
 "type": "object",
 "properties": {
8
 "name": {
9
 "type": "string"
10
11
 "email": {
12
 "type": "string"
13
14
 "shippingAddress": {
15
 "type": "string"
16
17
18
 },
 "required": [
19
20
 "name",
 "email",
21
 "shippingAddress"
22
23
 "additionalProperties": false
24
25
26
 </schema>
27
28 user
 We are registering 'Global Exports Ltd.' for your services. The main contact person
29
 is Samantha Davis, and her corporate email is s.davis@globalexports.co.uk. All ship-
 ments and correspondence should be directed to our headquarters: Global Exports Ltd.,
31
 12 Business Park Road, Manchester, M1 1AB, United Kingdom. We are looking forward to
32
 a fruitful partner ship and are particularly interested in your international ship-
33
34
 ping rates.
35
36 assistant
       ```json
```

Figure 9: Example prompt for the JSON task. The JSON schema in green is task-specific as well as the the user prompt in blue from which information should be extracted into the given schema. The system prompt and prefilled assistant response are fixed.

```
2 system
       You are a specialized AI assistant that generates SMILES (Simplified Molecular Input
3
       Line Entry System) strings from chemical descriptions. You will be given a textual
       description of a chemical compound or a related task. Your goal is to produce the
       most accurate and valid SMILES string representing that description.
      Your Task:
8
       Based on the provided "input" description, generate the corresponding SMILES string.
11
      Output Requirements:
12
13
       - Provide only the SMILES string as your output.
       - Ensure the SMILES string is syntactically valid.
15
       - Represent all specified chemical features accurately (atoms, bonds, rings,
16
           aromaticity, charge, isotopes, stereochemistry).
17
18
19
      Output:
20
       - Provide only the smiles molecule as a raw string between triple backticks (```).
21
22
       For instance:
       ```smiles
23
 C1=CC=CC=C1
24
25
26
27 user
 Propan-1-amine, a primary amine with a three-carbon straight chain and the amino
28
 group on the first carbon.
29
30
31 assistant
       ```smiles
```

Figure 10: Example prompt for the SMILES task. The user prompt in blue varies per task.

```
user
1
2
           Your goal is to create challenging and diverse `JSON Schema` problems. You are
           given a JSON schema that describes a specific schema for a JSON problem.
4
5
           You should generate **{num_samples}** JSON benchmark samples based on the
           provided schema. A benchmark sample consists of a natural language description
6
           describing how the JSON schema should be filled out, along with a JSON object
7
8
           that adheres to the schema.
9
           For each sample, provide a JSON object with the following structure:
10
11
           ```json
12
 {{
13
 "input": "A natural language description of how the JSON schema should be
14
15
 filled out. The input should be a natural query that a user might ask an
16
 LLM. The input will be given to the LLM as a prompt, along with the JSON
17
 schema. Based on this input, the LLM should generate a JSON object that
 adheres to the schema.",
18
 "output": "A JSON object that adheres to the provided schema. The output
19
 should be a valid JSON object that matches the schema and reflects the
20
21
 input description."
22
 }}
23
24
25
 Guidelines for generating samples:
26
 - **Variety**: Describe a wide range of scenarios that can be expressed using
27
 the JSON schema. Ensure that the samples cover a wide range of possible
28
 scenarios, and make them sound natural and plausible.
30
 - **Difficulty**: User queries can and should contain distracting information
 and longer backgrounds.
31
 - **Realism**: Test cases should reflect plausible scenarios where the JSON
32
 schema would be used.
33
 - **Reference**: Do not reference the JSON schema in the input description. The
34
 input should be a natural query that a user might ask an LLM. It should not
35
 reference JSON at all.
36
37
 JSON Schema:
39
 {schema}
40
 Example Input (Do not use this in your samples):
41
42
 {input_query}
43
 Example Output (Do not use this in your samples):
44
 {output_query}
45
```

Figure 11: Prompt used to generate additional JSON Schema samples for the JSON task using GEMINI-2.5-PRO. Several samples were generated at the same time to increase diversity.

```
1
 user
 You are a JSON Schema assistant. You will be given a textual description of how
2
3
 a JSON schema should be filled out. Your task is to generate a JSON object that
 adheres to the provided schema.
5
 Your Task:
7
 - Analyze the textual task.
 - Construct a JSON object that correctly implements the task based on the
 provided schema.
10
11
 The JSON object should be a valid JSON object that matches the schema and
12
 reflects the input description.
13
 Output:
14
 - Provide only the JSON object as a raw string between triple backticks
15
 (```json). Ensure the JSON object satisfies the JSON schema. For instance:
16
           ```json
17
           }}
18
           "key": "value",
19
20
           "number": 42,
           "array": [1, 2, 3]
21
22
23
24
25
           Json Schema:
26
           {schema}
27
           Description:
28
           {input_query}
```

Figure 12: Prompt used to verify additional JSON Schema samples for the JSON task using GEMINI-2.5-PRO.

```
1
      user
           You are a specialized AI assistant tasked with generating benchmark samples for
2
          SMILES (Simplified Molecular Input Line Entry System) string generation. Your
3
           goal is to create diverse and accurate chemical structure descriptions and their
           corresponding SMILES strings.
           Please generate **{num_samples}** benchmark samples.
7
8
           The difficulty of these samples should be: **{difficulty_description}**.
10
           Examples of difficulty levels:
           * **Beginner**: Simple acyclic molecules, common functional groups (e.g.,
11
               ethanol, acetic acid, propanamine), small alkanes/alkenes/alkynes.
12
13
           * **Intermediate**: Molecules with single or multiple rings (e.g., cyclohexane,
               pyridine, naphthalene), basic stereochemistry (R/S, E/Z using `@@`, `/`, `\`),
               common drugs or biomolecules (e.g., aspirin, glucose in its open-chain form).
15
           * **Advanced**: Complex polycyclic systems (e.g., steroids, bridged compounds),
16
17
               detailed stereochemistry, isotopic labeling, salts, mixtures, or reaction
18
               SMILES (if the task is to represent a reaction).
19
           For each sample, provide a JSON object with the following structure:
20
21
           ```json
23
 "input": "A natural language description of a chemical compound or a task that
24
 uniquely defines a chemical structure representable by a SMILES string.
25
 This could be an IUPAC name, a common name, a structural description, or
26
 a request to modify a base structure.",
27
 "output": "The correct and valid SMILES string for the chemical structure
28
 described in the 'input'. Correctness and validity are paramount."
29
30
 }}
31
32
 Guidelines for generating samples:
33
34
 - **Accuracy**: The generated SMILES string in the "output" field MUST
35
 accurately represent the chemical structure described in the "input". Ensure
 correct atom types, bond orders, connectivity, aromaticity, charges,
37
 isotopes, and stereochemistry as implied by the input.
38
39
 - **Validity**: All generated SMILES strings must be syntactically valid.
 - **Clarity of Input**: The "input" description should be unambiguous and
 provide enough information to define a specific chemical structure. Avoid
41
 overly vague descriptions.
42
 - **Variety**: Generate a diverse set of samples covering different chemical
43
44
 families, structural features (rings, unsaturation, heteroatoms, functional
 groups), and complexities according to the specified difficulty.
45
46
 Output Format:
47
48
 Return a JSON list containing the {num_samples} generated JSON objects.
```

Figure 13: Prompt used to generate additional samples for the SMILES task using GEMINI-2.5-PRO. Several samples were generated at the same time to increase diversity.

```
user
1
2
 You are a specialized AI assistant that generates SMILES (Simplified Molecular
 Input Line Entry System) strings from chemical descriptions. You will be given
 a textual description of a chemical compound or a related task. Your goal is
 to produce the most accurate and valid SMILES string representing that
5
 description.
6
 Your Task:
 Based on the provided "input" description, generate the corresponding SMILES
10
 string.
11
 Output Requirements:
13
14
 - Provide only the SMILES string as your output.
15
 - Ensure the SMILES string is syntactically valid.
16
 - Represent all specified chemical features accurately (atoms, bonds, rings,
17
 aromaticity, charge, isotopes, stereochemistry).
18
19
 Output:
20
 - Provide only the smiles molecule as a raw string between triple backticks (```).
22
23
 For instance:
           ```smiles
24
           C1=CC=CC=C1
27
28
           {sample}
```

Figure 14: Prompt used to verify samples for the SMILES task using GEMINI-2.5-PRO.