KNOWLEDGE-INFUSED DIAGRAMMING FEYNMAN: AGENT FOR SCALING VISUAL REASONING DATA 002

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ABSTRACT

Visual reasoning is an essential ability of state-of-the-art multi-modal AI systems. Improving these systems requires high-quality vision-language data at scale. Despite the abundance of internet image and text data, knowledge-rich and wellaligned image-text pairs are rare. In this paper, we present a scalable data generation pipeline built with our diagramming agent, FEYNMAN. To create diagrams, FEYNMAN first enumerates domain-specific knowledge components ("ideas") and performs code planning based on the ideas. Given the plan, FEYNMAN translates ideas into simple declarative programs and iterates to receives feedback and visually refine diagrams. Finally, the declarative programs are rendered by the PENROSE diagramming system. The optimization-based rendering of PENROSE preserves the visual semantics while injecting fresh randomness into the layout, thereby producing diagrams with visual consistency and diversity. As a result, FEYNMAN can author diagrams along with grounded captions with very little cost and time. Using FEYNMAN, we synthesized a dataset with more than 100kwell-aligned diagram-caption pairs. We also curate a visual-language benchmark, DIAGRAMMA, from freshly generated data. DIAGRAMMA evaluates the visual reasoning capabilities of vision-language models. We plan to release the dataset, benchmark, and the full agent pipeline as an open-source project.

1 INTRODUCTION

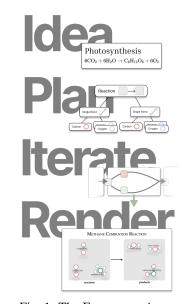


Fig. 1: The FEYNMAN Agent

A diagram is worth ten thousand words. Humans represent knowledge visually and solve complex problems efficiently using diagrams (Tversky, 2017; Larkin & Simon, 1987). However, the current generation of multi-modal large-language models (MLLMs) such as GPT-4V (Yang et al., 2023), Gemini (Team et al., 2023) and Llama 3 (Dubey et al., 2024b) still struggle to understand, use, and generate simple visual objects that often show up in diagrams, despite tremendous progress on general multi-modal benchmarks (Yue et al., 2024). Prior work have shown MLLMs to fail rudimentary vision tests (Rahmanzadehgervi et al., 2024), perceive graph structures poorly (Li et al., 2024d), and lack compositional understanding of visual attributes, relations, and ordering (Yuksekgonul et al., 2022). The important work (Zhang et al., 2024a) specifically demonstrated their weaknesses on reasoning with abstract mathematical diagrams.

Currently, training large models relies heavily on enormous amount of data for both pre- and post-training to make progress on any capabilities (Dubey et al., 2024a; Li et al., 2024c; Tong et al., 2024), including diagram understanding (McKinzie et al., 2024). To augment training data, one general strategy is to synthesize data using state-of-the-art large-language models. Unfortunately, synthesizing

vision-language data is challenging. Prevalent approaches of synthesizing vision-language data fo-051 cus on the language side, such as augmenting instruction-following data from image captions (Li 052 et al., 2022; Liu et al., 2024b; Wang et al., 2022). To synthesize images, the two main paradigms 053 are diffusion models (Rombach et al., 2022) and graphics program synthesizers (Belouadi et al.,

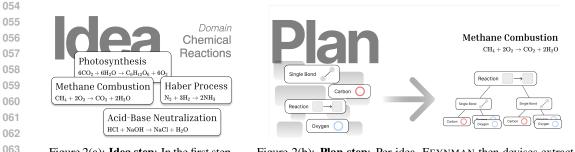


Figure 2(a): **Idea step**: In the first step, FEYNMAN enumerate the knowledge given a specific domain.

Figure 2(b): **Plan step**: Per idea, FEYNMAN then devises extract relevant elements such as chemical bonds and formulate a plan to translate them into Substance code.

2024b;c; Wu et al., 2023). The former generate raster images while the latter synthesize textual programs that produce vector graphics. Regardless of the output format, both approaches struggle to produce good diagrams consistently. Given the demand for high-quality synthetic diagrams and the limitations of current approaches, we ask the following research question:

Can we generate synthetic diagram-language pairs at scale?

When generating conceptual diagrams, models are tasked to perform both knowledge elicitation and 074 visual production. When prompted to produce a diagram representing some high-level concepts, the 075 model needs to elicit the relevant concepts (abstract knowledge, e.g., H₂O has 2 hydrogen and 1 076 oxygen atoms), map them to visual components (visual knowledge, e.g., use ball-and-stick model 077 to represent molecules), and organize these components in an image (visual production). However, 078 state-of-the-art diffusion and language models struggle because they are asked to perform these 079 steps all at once. For instance, diffusion models can produce visually pleasing images but may 080 ignore important concepts in the diagram; language models may include the right concepts in the 081 image but the diagram layout can be poor and illegible. In this paper, we recognize this challenge of 082 diagram generation, and ask:

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Can we decouple knowledge elicitation and visual production in diagram synthesis?

To address our questions, we elicit domain knowledge from LLMs and iteratively produce highquality diagrams using a knowledge-aware diagram interface. We propose FEYNMAN, an LLM agent that scales up diagram synthesis by decoupling knowledge elicitation and visual production. FEYNMAN leverages the knowledge advantage of modern LLMs by isolating knowledge elicitation 089 as its first step in diagram synthesis. Instead of directly producing SVG source code or a raster 090 image, FEYNMAN produces knowledge components ("ideas"), which are then translated to their 091 visual representations. To ensure high-quality visual production, FEYNMAN utilizes the PENROSE 092 language, which explicitly codifies the mapping from domain-specific concepts to their visual rep-093 resentations (Ye et al., 2020). The resulting diagram synthesis pipeline preserves the semantics of the diagrams, and we further utilize them to generate a diverse question-answer set tailored to the 095 generated content. Overall, our contributions include:

- 1. We created a diagramming agent, FEYNMAN, to author knowledge-infused diagrams and achieves remarkable yield rate in generating textbook-level diagram examples. Powered by PENROSE, FEYNMAN generates diagrams with diverse visual content.
- 2. With FEYNMAN, we generated 10693 knowledge-infused programs, leading to the creation of 106930 well-aligned diagram-caption pairs. This was accomplished within 1,550 million input and output tokens at a cost of under \$400 with GPT-40-mini.
- 3. We release a new benchmark DIAGRAMMA made of entirely fresh examples authored by FEYNMAN. We conducted a thorough quantitative evaluation of **17** MLLMs in Table 2
- 4. Via comprehensive ablations and analysis, we provide insights into how to build multi-modal AI agents that can work in the intersection of knowledge, visual design, and code generation. We analyze the economic aspects of synthesizing large-scale scientific diagrams using our pipeline.

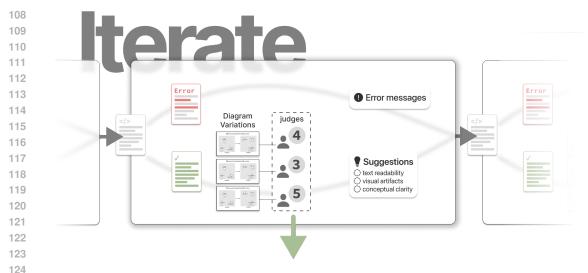


Figure 3: **Iterate Step**: At each step, FEYNMAN attempts to write PENROSE program to create a diagram. The generated program is then compiled into images and sent to a panel of visual judges (MLLMs) for critical feedback. We term this algorithm **Iterative Visual-Refine** (Algorithm 1).

Among prior work that explored similar directions, Belouadi et al. (2023) and Belouadi et al. (2024a) collected datasets of TikZ diagrams from the internet and arXiv articles to train coding agents for TikZ programs. AUTOMATIKZ (Belouadi et al., 2023) is an LLM coding agent that writes TikZ programs given text captions. However, after being trained with hundreds of thousands of TikZ diagrams scraped from arXiv IATEX sources, AUTOMATIKZ still exhibits efficiency overhead in synthesizing scientific diagrams at scale, due to the inherent complexity of both the TikZ language and visual design. In fact, both Belouadi et al. (2023) and Belouadi et al. (2024a) requires time-consuming tree search to boost compile success rates for simple programs, making large-scale generation infeasible. In general, there is still a lack of economical and scalable solution for generating diagrams embedded with rich knowledge.

2 DIAGRAMMING AGENT PIPELINE

In this section, we present the workflow of our diagramming agent, FEYNMAN. FEYNMAN's diagram synthesis pipeline includes four steps: **idea**, **plan**, **iterate**, and **render**. By leveraging the knowledge capacity of LLMs and a conceptual diagramming tool, FEYNMAN can generate grounded and diverse visual representations of scientific concepts at scale. Our pipeline has the following characteristics:

- 1. *Knowledge scalability*: Our choice to use an LLM to provide general "knowledge-focused planning" decouples the domain knowledge elicitation and the domain-specific visual design. This choice alleviates the cost of obtaining diverse and high-quality knowledge for the generation of domain-specific diagrams (Section 2.2).
- 2. *Visual diversity*: The optimization-based approach of the PENROSE rendering engine provides visual diversity even given the same visual concept (Section 2.1), boosting visual diversity of the synthesized diagrams.
- 3. *Image-text alignment*: The programs written by FEYNMAN simply encode the conceptual ideas and relationships, from which the visuals are automatically derived. These programs resemble natural language descriptions of the concepts, enabling smooth translation between concepts and code.

161 In this section, we first present the background of conceptual diagramming, which is the foundation of our approach, and then introduce each step in the agentic pipeline of FEYNMAN.



Figure 4: **Examples of conceptual diagrams and their** Substance **notations**: a graph where node connections form a cube (left) and the Lewis structure of the formaldehyde molecule (CH_2O).

2.1 BACKGROUND: CONCEPTUAL DIAGRAMMING

175 Conceptual diagrams refer to abstract images 176 that visually represent "a set of ideas and 177 their relations" (Tversky, 2017). At present, most conceptual diagrams are created by ei-178 ther a drawing tool like Adobe Illustrator or a 179 low-level graphical programming language like 180 PGF/TikZ or SVG. Using these tools is highly 181 manual and it is extremely difficult to use them 182 to automating diagram production (Ma'ayan & Ni et al., 2020). As a result, AI generation of 184 diagrams through TikZ has proved challenging 185 (Belouadi et al., 2023) (Fig. 7). 186

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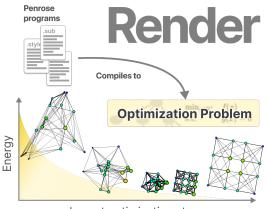
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PENROSE is a diagramming tool specifically 187 targeting conceptual diagrams. PENROSE sepa-188 rates the abstract concepts in the diagram (the 189 Substance) and the visual representations of 190 said concepts (the Style). Substance contains 191 no low-level visual details, it is simpler and eas-192 ier to generate correctly (Fig. 4). Style defines 193 a diverse space of *diagram variations* for any 194 given Substance. Combining Substance and



Layout optimization steps

Figure 5: FEYNMAN generates programs that PENROSE compiles to generate an layout optimization problem. The PENROSE layout engine then solves the optimization problem.

Style, PENROSE samples from this space when rendering a diagram, providing FEYNMAN the ability
 to produce many different examples even from just one set of concepts (Fig. 6).

197 To translate from concepts to visuals, Style converts the concepts and relationships from Substance 198 into a constrained optimization problem: every concept in substance is translated to one or more 199 shapes $\mathcal{S} = \{S_1, \ldots, S_n\}$, each with degrees of freedom $\vec{p} = (p_1, \ldots, p_m)$ such as width, height, 200 and center. Conceptual relations among concepts are translated to constraints and objectives: con-201 straints ensure that geometric predicates (e.g., contains, disjoint, etc.) hold true, while objectives encourage geometric relations to hold in the resulting diagram (e.g., shapes should be as far apart as 202 possible). PENROSE encodes constraints as nonnegative penalty functions $\mathcal{P}_1, \ldots, \mathcal{P}_l : \mathbb{R}^m \to \mathbb{R}_{>0}$ 203 each of which equal 0 if and only if the constraint is satisfied. Objectives are energy terms 204 $\mathcal{E}_1, \ldots, \mathcal{E}_k$. Overall, the PENROSE layout engine solves an optimization problem: 205

$$\min_{\vec{p}\in\mathbb{R}^m}\sum_{i=1}^k \mathcal{E}_i(\vec{p}) \quad \text{s.t.} \quad \sum_{i=1}^l \mathcal{P}_i(\vec{p}) = 0.$$
(1)

PENROSE employs an exterior point method (Hiroshi & Tanabe, 2010) to pose this problem as a sequence of unconstrained optimization problems, where constraints are iteratively stiffened over layout steps:

$$\min_{\vec{p} \in \mathbb{R}^m} \sum_{i=1}^k \mathcal{E}_i(\vec{p}) + c_n \sum_{i=1}^l \mathcal{P}_i^2(\vec{p}), \quad n = 0, 1, 2, \cdots$$
(2)

PENROSE solve this layout problem by running L-BFGS with line search (Lewis & Overton, 2009).

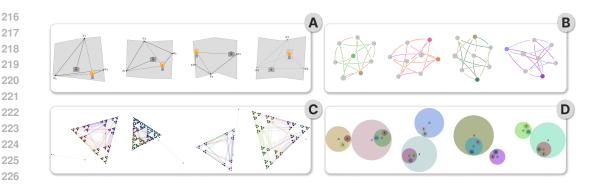


Figure 6: Diverse visual layouts of PENROSE diagram variations: using the same Substance, PENROSE can produce diagram variations while preserving the semantics, by sampling random initial values for shapes, colors, and other numerical quantities in the diagram. We show 4 random seed for 4 Substance programs for (A) ray-tracing diagrams, (B) Cayley graphs, (C) Chaos game as a Sierpinski triangle, and (D) Euler diagrams for sets.

2.2KNOWLEDGE PLANNING: ENUMERATING THE DOMAIN KNOWLEDGE WITH AN LLM

236 State-of-the-art LLMs learn vast knowledge during their large-scale pretraining. For example, GPT-237 40 attains 53% accuracy in the GPQA benchmark (Rein et al., 2023), close to the 57% achieved by human experts who have or are pursuing Ph.D. degrees. We leverage this large capacity of 238 knowledge of LLM by designing domain-specific prompts to ask an LLM to enumerate pieces of 239 knowledge ("ideas") related to the selected domain. The prompts are designed to encourage LLM 240 to perform creative knowledge enumeration. For example, LLM is given the question "Enumerate N chemical reactions that are pedagogical and important." in the chemical-reactions domain (see 242 examples of full domain planning prompts in Appendix B.2). We feed the LLM's response to the coding agent, FEYNMAN, to program the concepts into diagrams. In cases where we can't parse the 244 output format, we try multiple rounds until we reach a maximum number of rounds.

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- 2.3 DIAGRAMMING CODE PLANNING: REASONING FOR CONCEPTUAL DIAGRAMMING

248 In this stage, the FEYNMAN agent generates a coding plan for each of proposed knowledge compo-249 nents. The agent first attempts to organize the knowledge components into visual concepts, aiming 250 to prepare for translation into PENROSE code. To make the FEYNMAN agent aware of the PEN-251 ROSE syntax, we provide the official PENROSE documentation in the prompt, akin to Wu et al. 252 (2024a). Moreover, for each domain, we provide a few in-context examples for LLM to learn the 253 syntax for that specific domain. We then instruct FEYNMAN to plan the visual elements that are 254 described in each knowledge component. This involves listing important steps to write a Substance 255 program that corresponds to the sampled knowledge component (see full code planning prompts in Appendix B.4). Note that we do not instruct the model to write runnable code in this step, which is 256 257 an explicit design choice. In Section 4, we show that they serve as crucial foundations for successful and diverse code generation. 258

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2.4 ITERATIVE VISUAL-REFINE WITH A PANEL OF VISUAL JUDGES

262 After the planning stage, FEYNMAN translates the plan into compilable and correct PENROSE pro-263 grams. We found in our preliminary experiments that even though LLMs such as GPT-40 fail to write the correct program in their first attempt, they can improve if given suitable suggestions in 264 multi-round conversations. This is close to the interactive self-refine approach (Madaan et al., 265 2024), which improves LLM output quality via multi-round self-reflection. The refinement of dia-266 grams, which involves visual judgments, posed different challenges. While the prior work adopt tree 267 search to perform refinement (Belouadi et al., 2023; 2024a), their refinement process primarily aims 268 to achieve better compilation success rate. Without visual judgments and feedback, the generated 269 visual artifacts might include incorrect representation of knowledge.

270 To address this challenge, FEYNMAN utilizes a panel of visual judges to provide the visual feedback, 271 which we term it as **Iterative Visual-Refine**. The process is illustrated in Figure 3. In the first round, 272 FEYNMAN receives the plans from the previous planning steps and attempts to generate the first 273 code sample. If the code is successfully compiled into a diagram, then FEYNMAN run PENROSE to 274 generate variations of this diagram and send them to a panel of *visual judges* to assess its quality. 275 Each visual judge is a vision-language model asked to provide critical feedback to the diagramming 276 agent based on a set of *criteria* on various aspects of diagram qualities. To keep the task simple, we prompt the judges to answer in boolean values, which are then collected and aggregated. For 277 cost-saving purposes, we set a threshold of scores above which we accepts the output as a valid 278 diagram. We provide an aggregated feedback message and move to the next iteration if the program 279 generated arrives at any of these states: a) cannot be extracted from the LLM response; b) fail to 280 compile to diagrams or c) receive scores below the set threshold. The formal algorithm is presented 281 in Algorithm 1. 282

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284 De-duplication. LLM sometimes duplicate 285 their responses given similar prompts, result-286 ing in a lack of diversity of knowledge in dia-287 grams. Specifically, we focus on de-duplicating 288 the Substance code, which PENROSE uses to synthesize diagrams. We use a statement-wise Levenshtein distance (Levenshtein, 1966) to fil-290 ter programs that contain too many duplicate 291 statements. The detail is presented in Ap-292 pendix B.6. 293

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2.5 GROUNDED

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296 QUESTION-ANSWER PAIR GENERATION
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298 For each Substance code FEYNMAN generated, 299 we generate grounded captions from their code 300 programs, while diversifying its visual repre-301 sentation through the PENROSE optimization-302 based layout engine. We created a multiple-303 choice question-answering (QA) data generation pipeline. First, we generate image captions 304 305 by translating the concepts and relations in Substance to natural language. Then, we prompt an 306 LLM to select one of five visual reasoning skill 307 categories (Appendix B.7) for the problem. To 308 ensure problem diversity and quality, we ask the 309 model to provide rationales before QA genera-310 tion in a chain-of-thought fashion. Finally, after

Algo	rithm 1 Iterative Visual-Refine
	uire: Prompt S , Maximum iterations N_{max} ,
	Quality threshold θ , Number of Judges K
1: I	Initial Message: $S_0 \leftarrow S$
	$n \leftarrow 0$ {Initialize iteration counter}
3: 1	while $n \leq N_{\max}$ do
4:	Agent response $R \leftarrow \text{FEYNMAN}(S)$
5:	Parse R into PENROSE program C
6:	if Parsing returns no program then
7:	continue
8:	Compile C to diagrams $d_k, \forall k \in [K]$
9:	if Compilation Failure then
10:	Error: $e \leftarrow$ error traceback
11:	Message: $S \leftarrow e$
12:	continue
13:	for each $k \in [K]$ do
14:	Scoring: $s^{(k)} \leftarrow V_k(d_k)$
15:	Suggestions: $S^{(k)} \leftarrow V_k(d_k)$
16:	Average scores: $s_{n+1} \leftarrow Avg(s^{(k)})$
17:	Average suggestions: $S_{n+1} \leftarrow Avg(S^{(k)})$
18:	if $s_{n+1} \ge \theta$ then
19:	Exit the algorithm, returns C
20:	$n \leftarrow n+1$
21: 1	return C

a QA pair is generated, the model self-verify by checking if the question can be answered without an image and if the answer is correct given both image and question.

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2.6 BENCHMARK CURATION: THE DIAGRAMMA BENCHMARK

We curated DIAGRAMMA, a visual reasoning benchmark using diagrams FEYNMAN synthesized.
These diagrams are completely unseen and do not exist on the internet. DIAGRAMMA is a scientific
benchmark that contains 1,058 multiple choice questions of visual understanding and reasoning.
We manually filtered a synthetic test dataset generated by FEYNMAN to create DIAGRAMMA. We
went through a meticulous filtering process to ensure that the selected images had accurate labels,
correct knowledge representation, and sufficiently challenging questions. As shown in Table 1, DIAGRAMMA contains 6 subjects, each of which contains multiple subdomains e.g., sorting algorithms in computer science. Diagram counts for all subjects are listed in Table 2.

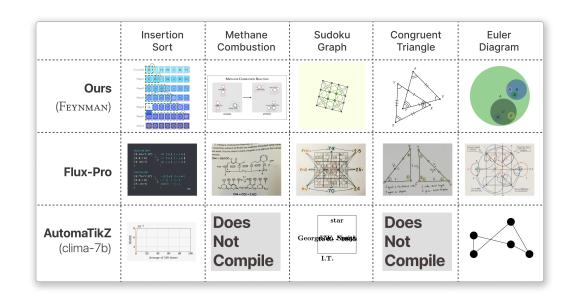


Figure 7: **Comparison of different diagramming approaches**: We select the best image out of three attempts using Flux-Pro and AUTOMATIKZ, compared with those generated by our agent. We provide them with the same prompt for each column. Flux-Pro produces visually diverse diagrams, however none of them contains legible text that matches the intent. AutomaTikZ, on the other hand, only successfully compiled for 3 out of 5 of all prompts.

3 EXPERIMENTS

3.1 SCALING DIAGRAM-CAPTION PAIRS

With the FEYNMAN agent, we conduct a preliminary dataset scaling experiment. By effectively enumerating knowledge in each subject and their subdomains, FEYN-MAN produced 10693 unique Substance programs, repre-senting diverse conceptual relationships. We used a total of 1470.4 million input tokens and 46.6 million output tokens on GPT-4o-mini to generate these Substance pro-grams. Each program is further independently rendered by the optimization-based layout engine to produce 10 unique variations, resulting in overall 106930 diagrams. See Figure 6 for examples of diagram variations and their visual diversity. For each rendered variation, we further produce a caption according to both the image and the corresponding Substance program. The scalability of the pipeline is tested in this experiment. In Appendix D.3, we provide more detailed studies to assess the knowledge and visual diversity of generated images.

Source metadata	
Subdomain	108
Substance	1058
Subjects	
Math	401 (37.9%)
CS	342 (32.3%)
Science	241 (22.8%)
Chart	30 (2.8%)
Common Sense	22 (2.1%)
Statistics	22 (2.1%)
Unique Style	52
Unique Domain	38

Table 1: Metadata of DIAGRAMMA.

3.2 DIAGRAMMA EVALUATION

We evaluated DIAGRAMMA on state-of-the-art open- and closed-source MLLMs. Evaluations were
 conducted in a zero-shot setting, with a uniform template provided to each model. Detailed evalua tion setup can be found in Appendix C.

Results. We present the evaluation results of DIAGRAMMA for a set of 17 models in Table 2. We observe three pieces of evidence validating our benchmark curation in the results: 1) as the sizes of models increase, their accuracy consistently improves, confirming the validity of our data for measuring the capabilities of MLLMs; 2) the computer science subject, which primarily involves graph

Model Name	All	Math	CS	Science	Chart	Commonsense	Statistics
Claude-3.5-Sonnet	59.64	64.59	42.98	74.69	53.33	77.27	54.55
GPT-40 (OpenAI (2024a))	57.28	63.09	50.58	60.17	53.33	50.00	36.36
Claude3-Opus (Anthropic (2024))	49.15	54.11	40.35	55.60	33.33	45.45	50.00
Gemini-1.5-Flash (Reid et al. (2024))	47.54	55.36	40.06	45.64	50.00	54.55	31.82
Claude3-Sonnet (Anthropic (2024))	47.54	50.62	38.01	58.92	46.67	36.36	27.27
GPT-4o-mini (OpenAI (2024a))	44.42	47.63	36.55	53.53	26.67	45.45	31.82
Gemini-1.5-pro (Reid et al. (2024))	44.23	49.13	41.23	42.74	30.00	59.09	22.73
Claude3-Haiku (Anthropic (2024))	42.53	46.63	31.58	54.77	30.00	36.36	27.27
Qwen2-VL-72B* (Yang et al. (2024a))	50.85	59.10	42.69	51.45	46.67	31.82	45.45
LLama3.2-VL-90B* (Dubey et al. (2024b))	46.88	50.37	41.23	53.53	26.67	40.91	31.82
LLama3.2-VL-11B (Dubey et al. (2024b))	46.22	48.38	40.06	56.02	30.00	50.00	13.64
Pixtral-12b*	44.71	50.62	40.06	44.81	43.33	36.36	18.18
LLava-OneVision-Qwen2-7b (Li et al. (2024b))	42.91	48.13	35.38	44.40	53.33	45.45	31.82
Qwen2-vl-7B (Yang et al. (2024a))	42.16	48.63	35.38	40.66	43.33	45.45	40.91
InternVL2-8B (Chen et al. (2024))	41.02	47.38	35.09	39.83	40.00	40.91	31.82
Phi-VL-3.5 (Abdin et al. (2024))	38.19	42.64	33.04	40.66	30.00	40.91	18.18
Minicpm-2.6 (Yao et al. (2024))	35.44	41.65	29.82	36.51	26.67	27.27	18.18

Table 2: Accuracy results of DIAGRAMMA on state-of-the-art MLLMs on **1058** samples. Models marked with (*) are evaluated through the OpenRouter API. **Claude-3.5-Sonnet** achieved the highest overall accuracy, with notable performance on science and commonsense diagrams.

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reasoning, remains the most difficult for current models, which corroborates with the observations by Li et al. (2024d); Rahmanzadehgervi et al. (2024). An notable observation is that Gemini-1.5 Flash, 400 which is considerably cheaper than Gemini-1.5 Pro outperformed Gemini-1.5 Pro on DIAGRAMMA, 401 a trend also seen in the reasoning category in LIVEBENCH (White et al., 2024). We conjecture this 402 correlation is attributed to that DIAGRAMMA share the same "freshness" as the reasoning questions 403 in LIVEBENCH. We find that Gemini 1.5 Pro declined to answer over 100 questions, contributing 404 to a more than 10% drop in accuracy, which might indicates high rejection rates of answering out-405 of-distribution questions. In Appendix C.4, we present a qualitative analysis of how most MLLMs 406 struggled in reasoning.

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4 ANALYSIS

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411 4.1 BASELINE COMPARISON

We show in Figure 7 a preliminary comparison study on 5 attempts to generate diagrams correspond-413 ing to specific prompts. We compare FEYNMAN to two competitors AUTOMATIKZ and diffusion 414 model FLUX-Pro (fal.ai, 2024) as baselines. Each attempt of baseline was ran 3 times and we se-415 lect the best result. The caption is provided in Appendix E.2. The diffusion model FLUX-Pro has 416 difficulty generating clean scientific diagrams that conveys the concepts, but instead hallucinates 417 many low-level details not mentioned in the caption. AUTOMATIKZ (Belouadi et al., 2023), which 418 trained a Llama-2 model to generate TikZ code, fails to produce correct TikZ programs that match 419 the captions. We hypothesize that their failure in our setting if because 1) complex diagrams require 420 great precision to draw than natural images, and 2) TikZ programs cannot separate knowledge or-421 ganization and visual production, which made the code synthesis task overly difficult. We provide 422 further explorations of using o1-mini and o1-preview (OpenAI, 2024b) to generate TikZ code in 423 Appendix E.2. However, even when powerful LLMs like o1-preview can write TikZ code roughly correctly, TikZ still makes it hard to diversify the layout. 424

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4.2 **PRODUCTION-TO-SCALE ANALYSIS**

We conducted an ablation experiment shown in Fig. 8 highlights the scalability of FEYNMAN. In
knowledge-dense domains, the agent scales its knowledge linearly as the number of tokens increases.
Even in knowledge-sparse domains, we observe an upward trend in token generation, though at a
reduced rate. This demonstrates the robustness of FEYNMAN 's performance across varying levels of domain.

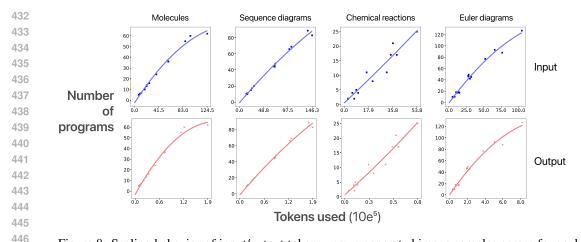


Figure 8: Scaling behavior of input/output tokens versus generated image samples across four sub domains. The figure illustrates two distinct trends: linear scaling in knowledge-dense domains, and
 decaying trends in knowledge-sparse domains. These trends highlight the impact of domain knowl edge diversity and scalability on the performance of FEYNMAN.

452 The results of our production-to-scale experiment on four selected subdomains are illustrated in Fig. 8. The plots show the total input/output tokens versus the number of generated images after 453 de-duplication. Across the domains, we observe two distinct scaling patterns: a linear trend and a 454 decaying trend. The linear trend suggests the potential for further scaling within a specific domain as 455 the number of tokens increases further. In contrast, the decaying trend indicates diminishing returns 456 in the generation of images as token counts continue to rise. We attribute these differing trends to 457 two main factors: (1) the base model's knowledge within the specific domain, and (2) the scalability 458 of the domain for diagramming. Additionally, domains can be classified as either knowledge-dense 459 or knowledge-sparse: for instance, enumerating knowledge about chemical reactions is likely easier 460 than for a domain composed solely of complementary triangles.

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4.3 ABLATIONS FOR AGENT WORKFLOW

To provide quantitative insights into the effectiveness of FEYNMAN, we evaluate our pipeline on two metrics: the final yield rate is percentage of successfully complied images after de-duplication; the visual judge scores is an average of rule-based critic score given by MLLM judges for de-duplicated images at the end of the generation. We perform an ablation study on 10 subdomains that encompass wide range of knowledge. As shown in Table 3, we ablate key components of FEYNMAN:
(1) explicit knowledge planing (KP, Section 2.2), (2) explicit code planning (CP, Section 2.3), and (3) early stop mechanism based on judge scores (S, Section 2.4).

471 We discuss three notable findings from our ablation results. First, the pipeline with all components 472 $(\mathbf{KP} + \mathbf{CP} + \mathbf{S})$ achieves the best average judge score. Second, code planning (CP), together with 473 use score to early stop, helps the generation pipeline end in much lower number of rollout rounds. Finally, when knowledge planning (**KP**) is present, the gap between compiled success rate and final 474 yield rate is very low. The observations above suggest that knowledge planning (KP) is essential for 475 generating diverse scientific diagrams. Additionally, code planning (CP) improves the scalability 476 of the data generation pipeline. When combined with early-stop, **CP** helps generate better-quality 477 figures with fewer iterations and reduce the overall cost. Combing both steps achieves our goal of 478 generating *scalable* and *diverse* diagrams.

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5 RELATED WORK

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Multi-modal LLMs and agents Vision-language models (Alayrac et al., 2022; Yang et al., 2023; Li et al., 2023a; Zhu et al., 2023) gained remarkable capability of following instructions through visual instruction tuning (Li et al., 2022; Liu et al., 2024b;a). This capability enabled wide range of applications, such as visual reasoning(Yue et al., 2024; Lu et al., 2023), and interact with human as

Ablations	Avg	PR	LT	SP	NR	CR	Compile %	Yield %	Rounds
KP + CP + S	65.4	69.7	30.9	60.4	91.8	74.2	82.5	82.5	2.63
CP + S	65.0	65.9	32.1	59.9	95.0	72.2	97.0	87.5	2.44
KP + S	62.8	63.9	35.6	56.8	91.3	66.2	87.0	86.5	6.69
S	63.2	64.3	31.5	57.6	90.6	71.8	96.5	84.0	6.29
KP + CP	61.5	67.9	25.9	52.1	89.7	71.9	81.5	81.5	8.00
СР	61.8	69.3	23.6	52.5	92.3	71.1	96.5	92.5	8.00
KP	63.9	66.6	32.1	59.5	91.2	70.2	87.5	87.5	8.00

Table 3: The table shows a break down of critic scores in five categories (see Appendix D.1, **PR**: proper element relationship; **LT**: legible text; **NR**: non-redundancy; **CR**: correct representation; **SP**: simplicity), diagram compilation rate (**Compile** %), final yield rate (**Yield** %), and total number of rounds in the iterate step (**Rounds**). The combination of explicit knowledge planning (**KP**), code planning (**CP**), and early stop based on scoring results (**S**) received the best judge critic score.

visual chatbots OpenAI (2024a). Meanwhile, agents built with LLMs can interact with environments
(Wang et al., 2024c) to play games, perform web navigation, and write computer programs (Wang et al., 2023; Yao et al., 2022; Romera-Paredes et al., 2024; Yang et al., 2024c; Xia et al., 2024;
Wu et al., 2024b). MLLM agents have more perception modalities and are more grounded in realworld scenarios (Hong et al., 2024; Sun et al., 2022; Li et al., 2024a; Wang et al., 2024a; Bonatti et al., 2024; Koh et al., 2024; Li et al., 2024e). Agents are also important collectors of data, but the efficiency of data collection depends on the domain of choice (Putta et al., 2024).

510 **Synthetic data generation** The success of large AI models depends primarily on the scaling law of 511 model size and training data (Kaplan et al., 2020; Hoffmann et al., 2022), which stimulated efforts 512 to curate datasets (Gao et al., 2020; Soboleva et al., 2023; Li et al., 2024c). For domains where 513 data collection is expensive, synthesizing data has become the dominant approach (Haluptzok et al., 514 2022; Zelikman et al., 2022; Yang et al., 2024b; Li et al., 2023b; Wang et al., 2022; Peng et al., 2023). 515 Synthetic data have long existed in the vision domain (Little & Verri, 1989). For multi-modal AI 516 models, teaching the model to harness their visual reasoning capabilities also relies on synthetic data (Li et al., 2022; Liu et al., 2024b;a). One work that tackled similar problems to ours is by Zhang 517 et al. (2024b), who synthesized charts and figures via LLM knowledge and program synthesis, but 518 their approach is limited by the tool of choice and lack of agentic ability such as iterative refinement. 519

520 Vision-language benchmarks Sustainable progress of AI research relies on the continuous de-521 velopment of benchmarks to measure the capabilities of AI systems. Benchmarks like HellaSwag 522 (Zellers et al., 2019; Hendrycks et al., 2020; Cobbe et al., 2021; Zheng et al., 2023) contributed sig-523 nificantly to the progress measurement of building state-of-the-art LLMs. Vision-language bench-524 marks serve the same role for the visual understanding and reasoning abilities of MLLMs. For exam-525 ple, benchmarks like VQA-v2 (Antol et al., 2015), GQA (Hudson & Manning, 2019) and MMMU 526 (Yue et al., 2024) measure the visual knowledge of MLLMs comprehensively. Other benchmarks 527 like (Methani et al., 2020; Lu et al., 2021b;a; Masry et al., 2022; Lu et al., 2024; Wang et al., 2024b) 528 measure domain-specific capabilities like chart understanding and math visual reasoning.

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6 CONCLUSION

532 In this paper, we presented FEYNMAN, a diagramming agent that authors conceptual diagrams at 533 scale. FEYNMAN decouples knowledge elicitation from visual production of diagrams to achieve 534 scalability of diagram synthesis. Grounded by a knowledge-infused diagramming language, FEYN-535 MAN produces text-image pairs to scale up the synthetic data across multiple subjects, such as com-536 puter science and mathematics. We conducted systematic ablation of key design choices for FEYN-MAN, and showed the production-to-scale curves to demonstrate the scalability of our pipeline. 537 Additionally, we released a new benchmark DIAGRAMMA with question-answer pairs generated 538 by FEYNMAN and curated to ensure correctness, further contributing to research in diagram-based 539 reasoning.

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inddef's effectiveness in domains where LLMs have incomplete of blased knowledge, resulting in
 less diverse outputs. A key area for future work is improving how knowledge is elicited from LLMs.
 For example, this may involve integrating a Retrieval-Augmented Generation (RAG) pipeline to
 supplement LLMs with external, domain-specific information.

Limited Diagram Style Variation: While the generated diagrams exhibit layout diversity, control over stylistic elements, such as color schemes or visual aesthetics, is limited to the default capabilities of the PENROSE language. To address this, future efforts will focus on systematically varying Style and Domain programs in PENROSE, enabling more flexible and customizable diagram generation.

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B DETAILED PIPELINE FOR FEYNMAN

- **B.1** PIPELINE CONFIGURATION
- Below we create a list of hyperparameters used in FEYNMAN. An ablation study is done in Section 4 on some key hyperparameters, labeled with (*).

864	Planning LLM: the model used during Knowledge Planning section
865	• Coding LLM: the model used during Code Planning and Generation
866 867	 Number of Rounds: The number of iterative improvement rounds per sample
868	• Critic MLLMs: a list of MLLM candidate used to judge the image at the end of each
869	rollout rounds and final generation pipeline
870	• Use Knowledge Planning*: A flag to note whether to explicitly conduct one turn of knowl-
871	edge planning conversation
872	• Use Code Planning*: A flag to note whether to explicitly conduct one turn of code plan-
873	ning conversation
874	• Use Scores to Early Stop*: A flag to note whether to use critic MLLM judge score to
875	early exit rollout. If the flag is set to false, the code model only receives MLLM feedback.
876 877	
878	The default configuration for FEYNMAN is to use GPT-40 as the planning model and GPT-40-mini
879	as coding LLM. Our MLLM candidates are selected from GPT-4o-mini, Claude-3.5-sonnet, and
880	Gemini-1.5-Pro. The number of rollout rounds are set to 8, with all flags set to true.
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918 **B.2** PROMPT FOR KNOWLEDGE PLANNING 919

In this section, we provide knowledge planning prompts in some example domain. These prompts aim to encourage LLM's to elicit its pretrain knowledge to think of creative scenarios in a given domain, specially for elements that can be altered through substance code.

Geometry:

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As a geometry teacher, think of various ways to draw geometric shapes and their constructions with clear labeling. Your goal is to help students understand the properties and relationships of geometric figures through detailed and thoughtfully designed diagrams. Outline a variety of diagrams that could be drawn in this domain. Guidelines:

1. Concept Focus:

- Shape Types: Utilize various shapes like triangles, quadrilaterals, rectangles, circles, and angles to demonstrate different geometric principles.

- Geometric Constructions: Show constructions such as bisectors, perpendicular bisectors, midpoints, and angle formations to illustrate fundamental concepts.

 Relationships and Properties: Highlight geometric relationships and properties such as parallelism, equal lengths, and angle measures.

2. Planning Elements:

- Diagram Layout: Decide on the arrangement of shapes and lines to clearly show their relationships and constructions. Consider layouts that logically progress through the steps of construction.

- Labeling: Plan to consistently and clearly label all points, lines, and angles to enhance understanding. Ensure labels do not clutter the diagram and are easily readable.

Word Cloud:

As a high school English teacher, generate engaging word clouds to help students visualize key concepts in literature. Word clouds should highlight word frequency and importance to aid understanding of themes, vocabulary, and literary devices.

Guidelines:

1. Focus on concepts like themes, important vocabulary, literary devices, and text analysis.

2. Use texts appropriate for high school students, exclude common stop words, and design for readability and appeal.

3. Ensure significant words are prominent and visuals accurately reflect word emphasis. 4. Examples:

- Word cloud of common words in a Shakespearean soliloguy.

- Word cloud highlighting key vocabulary from a novel chapter.

- Word cloud showcasing sensory words in a descriptive essay.

5. Keep word clouds simple, use them to prompt discussions, and include brief annotations or questions to encourage critical thinking.

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972	Matrix Operation:
	As a mathematics teacher focusing on matrix operations, design a variety of diagrams
974	to illustrate fundamental matrix and vector operations. Your goal is to help students
975	understand the essential principles and applications of matrix operations through
976	thoughtfully designed diagrams. Outline a range of diagrams that could be drawn in this
977	domain. Guidelines:
978	
979	1. Concept Focus:
980	- Basic Elements: Represent scalars, vectors, and matrices to demonstrate foundational
981	concepts.
982	- Matrix and Vector Operations: Highlight important operations such as transposition,
983	scalar multiplication, matrix multiplication, vector addition, and element-wise operations.
984	- Applications: Optionally illustrate applications of matrix operations in solving linear
985	equations, transformations, and other practical scenarios.
986	
987	2. Planning Elements:
988	- Diagram Layout: Arrange matrices, vectors, and scalars clearly to show their relation-
989	ships and operations. Consider using simple, clean layouts to avoid confusion.
990	- Labeling: Clearly label all elements (matrices, vectors, scalars) and their components for easy identification. Use consistent and concise labeling throughout the diagrams.
991	for easy identification. Use consistent and concise labeling throughout the diagrams.
992	
993	3. Diverse Diagrams Examples:
994	- Transpose of a Matrix: Draw a matrix and its transposed version to illustrate the
995	concept of matrix transposition.
996	- Scalar Multiplication: Show examples of scalar multiplication with matrices and vectors,
990 997	demonstrating how each element is scaled.
997 998	, and the second s
	4. Educational Focus:
999	- Clarity: Ensure each diagram is easy to interpret and effectively clarifies matrix
1000	operations concepts for students. Strive for simplicity and avoid unnecessary complexity
1001	in the diagrams.
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1003	Use these guidelines to outline a series of well-organized and informative diagrams
1004	that will effectively aid in teaching the principles and applications of matrix operations.
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1027	Chemistry Structural Formula:
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1029 1030	As a high school teacher in chemical synthesis and reaction design, I need your help to generate novel and potentially useful chemical reactions. Please follow these guidelines:
1031 1032 1033 1034 1035 1036	 Consider various types of organic and inorganic reactions, including but not limited to: Carbon-carbon bond formations Oxidation and reduction reactions Substitution reactions
1037 1038 1039 1040 1041 1042 1043	 2. Take into account different reaction conditions such as: - Temperature ranges - Pressure conditions - Solvents - Catalysts - pH levels
1044 1045 1046 1047 1048 1049	 3. For each proposed reaction: Provide the balanced chemical equation Suggest possible reaction mechanisms Describe the expected products and any significant side products Explain the potential significance or applications of the reaction
1050 1051 1052	Please write down the formula of the reactants and products in the chemical re- action.
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1080 **B.3** PROMPT TO SCALE KNOWLEDGE PLANNING PROMPTS 1081

1082 The prompt includes few-shot examples across various related domains, each with a corresponding 1083 PENROSE domain code and a manually crafted prompt. The domain code is provided as it best 1084 captures key knowledge elements essential to image construction in PENROSE, making it the most 1085 relevant information to include in a knowledge planning prompt.

Create a prompt that encourages the model to generate creative scenarios within a specific domain. The prompt should guide the model to identify scalable knowledge elements in that domain and ensure the output is clear and easy to understand. Here are a few examples:

Example Domain 1: {example domain name 1}

Example Domain Code 1: {example Penrose domain code 1}

Example Domain Prompt 1: {example domain knowledge planning prompt 1}

Example Domain 2: {example domain name 2}

Example Domain Code 2: {example Penrose domain code 2}

Example Domain Prompt 2: {example domain knowledge planning prompt 2}

Example Domain 3: {example domain name 3}

Example Domain Code 3: {example Penrose domain code 3}

Example Domain Prompt 3: {example domain knowledge planning prompt 3}

Now generated knowledge planning prompt for the given domain name and code

Domain name: {domain name}

Domain code: {domain code}

Domain Prompt:

1	1	0	7
1	1	0	8
1	1	0	9
1	1	1	0
1	1	1	1
1	1	1	2
1	1	1	3
1	1	1	4
1	1	1	5
1	1	1	6
1	1	1	7
1	1	1	8
1	1	1	9
1	1	2	0
1	1	2	1
1	1	2	2
1	1	2	3
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1	1	2	6
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1	1	3	0

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1134B.4PROMPT FOR CODE PLANNING1135

{domai	n_instructions}
	give you the domain definition, and the corresponding domain code. You
	o refer to the documentation of the domain and substance in penrose for deeper
underst	anding.
Domair	n documentation: {documentation_content}
Now he	ere is an example of the substance code in this domain for{domain_name}:
cubetan	<pre>ice:{substance_code_shot_content}</pre>
Substan	
Given	your planning above, please plan a few important steps for generating the
substan	ice code for {idx}-th example given the domain and style.
Doviou	the plan provided and ensure a clear understanding of each stop. Pofere
	the plan provided and ensure a clear understanding of each step. Before ing the code, think through the following:
general	ang the code, think through the following.
1. Enlis	st the components of the particular example.
2. How	does each step translate into the penrose substance code?
\A/ ··	
	down the reasoning and the steps you will take, especially the elements
uenned	in the domain you will put on the diagram and the relations between them.
e promp	t includes several key Python formatting elements:
· r · r	
	omain Instructions: Hand-crafted instructions specific to code generation within a
	omain. For example, in the geometry domain, these instructions may guide the model to
	e concise labeling for each shape.
	ocumentation content: Relevant PENROSE documentation, primarily covering syntax r domain, substance, and style code.
• Su	ubstance code shot content: Example compilable substance codes from the same
do	omain, sourced either from the official PENROSE repository ¹ or previous successful itera-
tic	ons.
¹ https:/	//github.com/penrose/penrose/tree/main/packages/examples/src

1188 B.5 MULTI-JUDGE CRITICS

For each round, we have a number of MLLM judges to assess the quality of compiled images based on pre-defined criterion. Our candidate judges are GPT-40, Claude-3.5-sonnet, Gemini-Pro-1.5. Each judge is randomly selected from candidate pool with a different random seed. The criterions are listed as follows:

- Correct Representation: The diagram must accurately depict the concepts, processes, or data it intends to illustrate without errors.
 - Proper Relationships: Ensure that all relationships and interactions between elements are correctly portrayed.
 - Legible Text: If there is any labels, legends, and annotations, then they should be easily readable. Long labels and annotations should be avoided.
 - Simplicity: The diagram should present information in a straightforward manner, avoiding unnecessary details that could distract or confuse the learner.
 - Cultural Sensitivity: Avoids symbols or imagery that might be culturally insensitive or misunderstood by the target audience.
 - Organized Structure: Elements should be arranged logically to guide the reader's eye through the information seamlessly.
 - No Unnecessary Repetition: Ensures that each element serves a purpose without redundant information that could clutter the diagram.

You are given one diagram generated by the user via graphics programs. The creative intent of the diagram is:

{diagram_intent}

Do you think the diagram preserves the creative intent well? Please evaluate the validity of the diagram based on the following criteria, and provide a short suggestion for improvement at the end:

{criterion}

Format your answer as follows:

Comment: [YOUR COMMENT]

Correct Representation Criterion Satisfied: If you think the criterion is satisfied, say yes $\langle GOOD \rangle$, if not, say no $\langle BAD \rangle$. Proper Relationships Criterion Satisfied: If you think the criterion is satisfied, say yes $\langle GOOD \rangle$, if not, say no $\langle BAD \rangle$. Legible Text Criterion Satisfied: If you think the criterion is satisfied, say yes $\langle GOOD \rangle$, if not, say no $\langle BAD \rangle$. Simplicity Criterion Satisfied: If you think the criterion is satisfied, say yes $\langle GOOD \rangle$, if not, say no $\langle BAD \rangle$. Simplicity Criterion Satisfied: If you think the criterion is satisfied, say yes $\langle GOOD \rangle$, if not, say no $\langle BAD \rangle$. Cultural Sensitivity Criterion Satisfied: If you think the criterion is satisfied. If you think the criterion Satisfied. If you think the criterion Satisfied: Say yes $\langle GOOD \rangle$, if not, say no $\langle BAD \rangle$. No Unnecessary Repetition Criterion Satisfied: If you think the criterion is satisfied, say yes $\langle GOOD \rangle$, if not, say no $\langle BAD \rangle$. No Unnecessary Repetition Criterion Satisfied: If you think the criterion is satisfied, say yes $\langle GOOD \rangle$, if not, say no $\langle BAD \rangle$.

Suggestions: [YOUR SUGGESTIONS]

The format instruction allows us to use the following regex code to parse the binary score (1 for good, 0 for bad). A total score is calculated based on average score for each judge.

1240
score_pattern = r"(?i)<(good|bad)>"
1241
suggestion_pattern = r"(?i)\bsuggestion[s]?:\s*(.*)"

1242 B.6 DE-DUPLICATION DETAILS

1244 During de-duplication, we focus on filtering similar substance codes within the same domain. Bor-1245 rowing the idea from Levenshtein distance, for each new substance code s and existing set of final 1246 substance **S**, we determine whether to add s to **S** based on the following algorithm

	rithm 2 Determine whether to add sample s to set S based on threshold T
Reau	
	ire: Sample s, Set of samples S, Similarity threshold T
	re: Decision to add s to S (True or False)
	or each $s' \in \mathbf{S}$ do
2:	Split both s and s' into lines Sort lines of s and s'
3: 4:	Compute Levenshtein distance d between lines of s and s'
5:	if $d > T$ then
6:	return False
7: 1	eturn True
3.7	QUESTION ANSWER GENERATION SKILL CATEGORY
fo	isual Recognition: Ask about recognition of the elements in the diagram. You can a or sophisticated visual recognition, such as counting a type of elements, or the numb
0	f elements with a certain property.
tl	rithmetic Calculations: Ask about arithmetic calculations based on the description ne diagram, such as addition, subtraction, multiplication, division, or quantities compa on. Ask questions about basic asthmatics reasoning using the elements in the substance
	cientific Knowledge: Ask questions about the scientific knowledge that a
	ontained in the diagram. Ask questions that test understanding of these knowled ased on the diagram.
	ased on the diagram.
D	
	patial Relationships: Ask questions about the spacial relationships between t
S	patial Relationships: Ask questions about the spacial relationships between the ements in the diagram.
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1296 B.8 QUESTION ANSWER GENERATION DETAILS

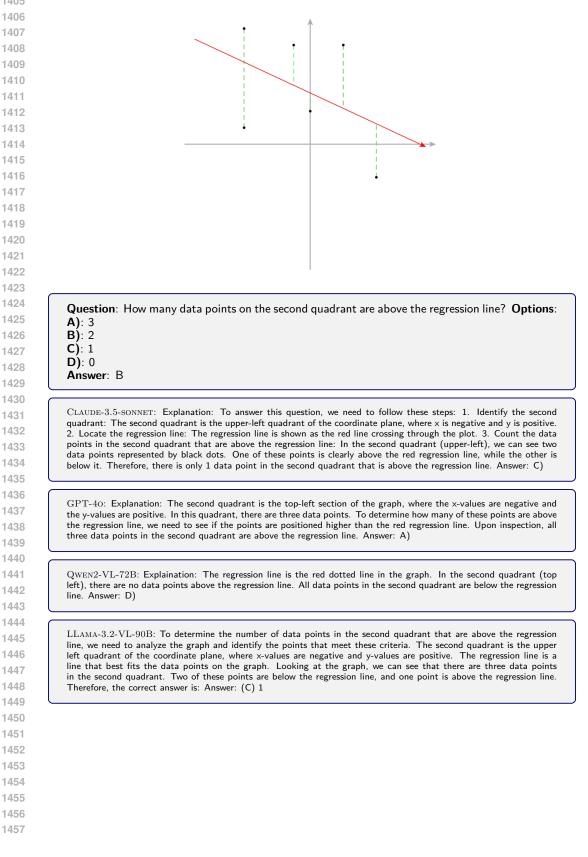
98 99 800	
	Your job is to generate multiple-choice questions and answers based on the given
00	diagram, substance code, and description. There is the (code and text) description of
801	a diagram: context. Given the information in the description, generate a multiple-choice
802	question answer pair which has 4 labeled as A, B, C, D. You should take the following
803	steps to generate the question:
804	1. This has a backlish of a sector of a structure of the sector of the s
805	1. Think about what kind of question you can ask. Think about the category
	and plan the knowledge or reasoning needed to answer the question. 2. Provide the
806	reasoning of the questions and the rationale for the correct answer, and then present the
807	question, options and answer using the following template. 3. Refer to the elements via
808	labels in the substance code and ensure that the question can be answered with the image.
809	
10	Here is an example multiple-choice question answer template:
811	
12	{format_template}
13	
814	Guidelines: 1. Don't reveal all the information about the diagram in the ques-
	tion, demand the test taker to look at the diagram to answer the question to extract
15	necessary information. 2. The substance code defined all the elements and relationships
16	in the diagram, but it is hidden from the test taker. You should only ask questions
817	about elements and relationships in the image. For example, you should refer to the
18	elements defined in "'AutoLabel"' in the substance code. Anything that is not in the
19	image should not be asked in the question. 3. Don't ask questions about font size,
20	pixels, hyper-parameters or any information not shown in the image.
1	
2	{past_questions_prompt}
3	
4	{skill_category_prompt}
	Now please generate a multiple-choice question and the corresponding options
	and answer.
	Above shows the prompt for generating multiple choice questions. There are several key elements
	input as string formatting. They are listed below:
	• Context: This include both the image and PENROSE substance code.
	• format_template: this is a format template passed to model so that we could use regex to
	parse the generated questions and answers.
	purse the generated questions and answers.
	• skill_category_prompt: a skill category is randomly chosen. In addition to the category
	• skill_category_prompt: a skill category is randomly chosen. In addition to the category
	• skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category.
	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves
	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves
Г	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication.
ſ	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication.
	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication. The regex code used to parse the generated questions and answers are provided below: question_pattern = re.compile(r'question\s*\d*:\s*(.*?)(?=\n[A-D]\))', re
[skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication. The regex code used to parse the generated questions and answers are provided below: question_pattern = re.compile(r'question\s*\d*:\s*(.*?)(?=\n[A-D]\))', re .DOTALL re.IGNORECASE)
	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication. The regex code used to parse the generated questions and answers are provided below: question_pattern = re.compile(r'question\s*\d*:\s*(.*?)(?=\n[A-D]\))', re .DOTALL re.IGNORECASE) option_pattern = re.compile(r'\n([A-D])\)\s*([^\n]+)')
	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication. The regex code used to parse the generated questions and answers are provided below: question_pattern = re.compile(r'question\s*\d*:\s*(.*?)(?=\n[A-D]\))', re .DOTALL re.IGNORECASE) option_pattern = re.compile(r'\n([A-D])\)\s*([^\n]+)') rational_pattern = re.compile(r'Reasoning\s*:\s*(.*)')
	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication. The regex code used to parse the generated questions and answers are provided below: question_pattern = re.compile(r'question\s*\d*:\s*(.*?)(?=\n[A-D]\))', re .DOTALL re.IGNORECASE) option_pattern = re.compile(r'\n([A-D])\)\s*([^\n]+)') rational_pattern = re.compile(r'Reasoning\s*:\s*(.*)')
	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication. The regex code used to parse the generated questions and answers are provided below: question_pattern = re.compile(r'question\s*\d*:\s*(.*?)(?=\n[A-D]\))', re .DOTALL re.IGNORECASE) option_pattern = re.compile(r'\n([A-D])\)\s*([^\n]+)') rational_pattern = re.compile(r'Reasoning\s*:\s*(.*)') category_pattern = re.compile(r'(?i)(?<=\W)\nanswer(?=\W).*?\b([A-D])\)\s
	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication. The regex code used to parse the generated questions and answers are provided below: question_pattern = re.compile(r'question\s*\d*:\s*(.*?)(?=\n[A-D]\))', re .DOTALL re.IGNORECASE) option_pattern = re.compile(r'\n([A-D])\)\s*([^\n]+)') rational_pattern = re.compile(r'Reasoning\s*:\s*(.*)')
	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication. The regex code used to parse the generated questions and answers are provided below: question_pattern = re.compile(r'question\s*\d*:\s*(.*?)(?=\n[A-D]\))', re .DOTALL re.IGNORECASE) option_pattern = re.compile(r'\n([A-D])\)\s*([^\n]+)') rational_pattern = re.compile(r'Reasoning\s*:\s*(.*)') category_pattern = re.compile(r'(?i)(?<=\W)\nanswer(?=\W).*?\b([A-D])\)\s
	 skill_category_prompt: a skill category is randomly chosen. In addition to the category itself, the model receives the description of the selected category. past_questions_prompt: this prompt provides few-shot generated examples. It serves both as shot examples and de-duplication. The regex code used to parse the generated questions and answers are provided below: question_pattern = re.compile(r'question\s*\d*:\s*(.*?)(?=\n[A-D]\))', re .DOTALL re.IGNORECASE) option_pattern = re.compile(r'\n([A-D])\)\s*([^\n]+)') rational_pattern = re.compile(r'Reasoning\s*:\s*(.*)') category_pattern = re.compile(r'(?i)(?<=\W)\nanswer(?=\W).*?\b([A-D])\)\s

2.1	EVALUATION HYPERPARAMETER
his	section contains the hyperparameter for evaluation.
	• Temperature: the temperature of generation for both closed source and open sourced are set to 0 .
	 Maximum new token: this parameter is the max generation length for close sourced a For models from huggingface, this refers to the max_new_token parameter in ger config. This value is set to 512 for open sourced models, and 2048 for close a models.
	• Batch size: this refers to input batch size for open sourced models and parallel nur processes for close sourced models. This is set to 16 for close and open sourced models.
	• Chat template: the formatting for all models used follow their official document of gingface example.
	• Image size: All of our default image sizes are 600 × 600 pixels. For API-based minages are fed to models directly. For open-sourced models, images are resized to 384 pixels first.
2.2	EVALUATION PROMPT
F	Please provide a detailed explanation to your solution, and, in the last line, conclude y
F a a	Please provide a detailed explanation to your solution, and, in the last line, conclude y inswer with a specific label (A, B, C, D) that corresponds to the correct answer. Her
F a a E	Please provide a detailed explanation to your solution, and, in the last line, conclude y inswer with a specific label (A, B, C, D) that corresponds to the correct answer. Her in example answer:
F a a E	Please provide a detailed explanation to your solution, and, in the last line, conclude your solution, and, in the last line, conclude yourswer with a specific label (A, B, C, D) that corresponds to the correct answer. Herein example answer: Explanation: <your explanation=""> Answer: <your answer=""></your></your>
F a a E <i>F</i> M	Please provide a detailed explanation to your solution, and, in the last line, conclude yourswer with a specific label (A, B, C, D) that corresponds to the correct answer. Herein example answer: Explanation: <your explanation=""> Answer: <your answer=""> Now answer the question based on the diagram</your></your>
F a a E <i>F</i> M	Please provide a detailed explanation to your solution, and, in the last line, conclude your solution, and, in the last line, conclude yourswer with a specific label (A, B, C, D) that corresponds to the correct answer. Herein example answer: Explanation: <your explanation=""> Answer: <your answer=""></your></your>
F a a E <i>F</i> M	Please provide a detailed explanation to your solution, and, in the last line, conclude yourswer with a specific label (A, B, C, D) that corresponds to the correct answer. Herein example answer: Explanation: <your explanation=""> Answer: <your answer=""> Now answer the question based on the diagram</your></your>
F a a E <i>F</i> M	Please provide a detailed explanation to your solution, and, in the last line, conclude yourswer with a specific label (A, B, C, D) that corresponds to the correct answer. He in example answer: Explanation: <your explanation=""> Answer: <your answer=""> Now answer the question based on the diagram Question: {Question}</your></your>
F a a E A M C C.3	Please provide a detailed explanation to your solution, and, in the last line, conclude inswer with a specific label (A, B, C, D) that corresponds to the correct answer. He in example answer: Explanation: <your explanation=""> Answer: <your answer=""> Now answer the question based on the diagram Question: {Question} Answer:</your></your>

C.4 FINE-GRAINED COMPARATIVE ANALYSIS

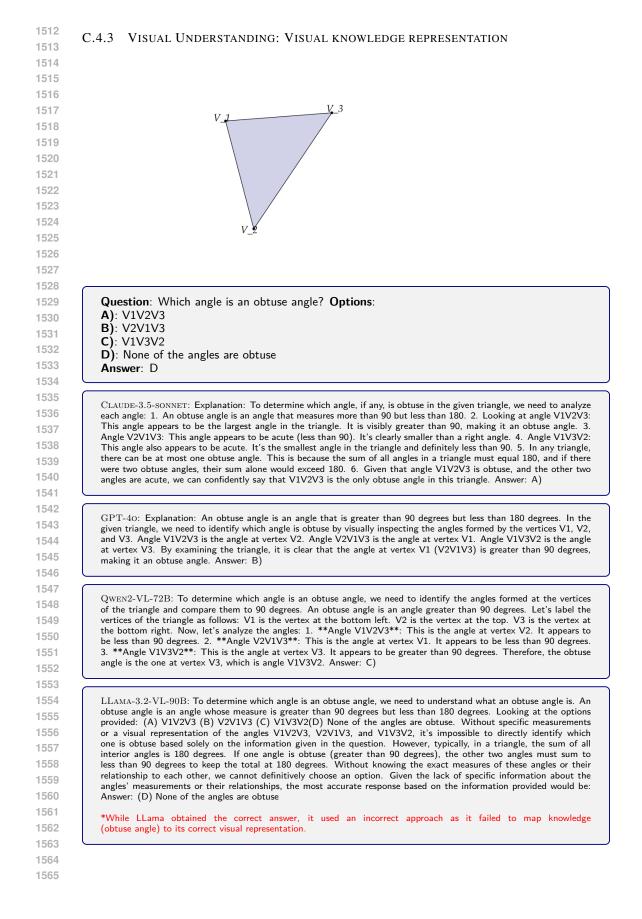
In this section, we prove some examples in DIAGRAMMA where top two open-sourced and close-sourced models both failed. The candidates are CLAUDE-3.5-SONNET, GPT-40, QWEN2-VL-72B, LLAMA-3.2-VL-90B. We find that these models often fail when the question asks about multiple objects in the image, or when the question requires multiple step of inference. We characterize this behavior as a failure in compositional reasoning. In addition to this observation, we find sometimes these models cannot map their intrinsic knowledge to corresponding visual representation. We will give examples to both failures in the following pages.

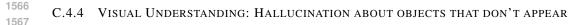


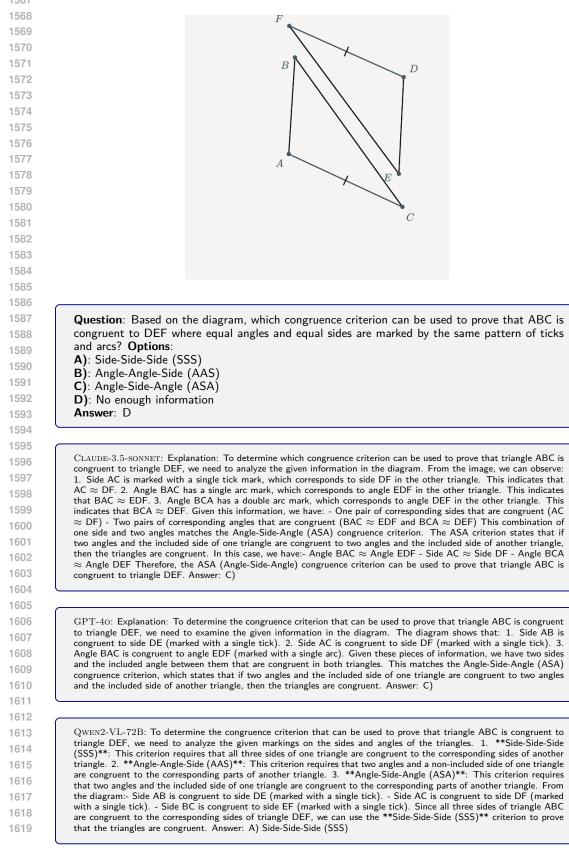




1458 C.4.2 COMPOSITIONAL REASONING: MULTI-OBJECT INFERENCE







 $\rm LLAMA-3.2-VL-90B$: To determine the congruence criterion for proving that triangle ABC is congruent to triangle 1621 DEF, we need to analyze the given information in the diagram. 1. **Identify Equal Sides and Angles**: The diagram 1622 shows that side AB is equal to side DE (indicated by the same pattern of ticks) and angle BAC is equal to angle EDF (indicated by the same pattern of arcs). Additionally, side BC is equal to side ÉF (same pattern of ticks). 2. **Apply Congruence Criteria**: - **SSS (Side-Side-Side)**: This criterion states that if three sides of one triangle are equal 1623 to three sides of another triangle, then the two triangles are congruent. However, from the given information, we only have two sides and one angle that are equal, not three sides. - **AAS (Angle-Angle-Side)**: This criterion requires 1624 1625 two angles and a side of one triangle to be equal to two angles and a side of another triangle. The given information 1626 matches this criterion because we have two equal angles (angle BAC = angle EDF) and one equal side (AB = DE). **ASA (Angle-Side-Angle)**: This criterion requires two angles and the included side of one triangle to be equal 1627 to two angles and the included side of another triangle. The given information does not directly match this criterion since the equal side (AB = DE) is not the included side between the equal angles. 3. **Conclusion**: Based on the 1628 analysis, the congruence criterion that can be used to prove that triangle ABC is congruent to triangle DEF is AAS 1629 (Angle-Angle-Side), as it matches the given equal angles and side in the diagram. **Answer: B) 1630 1632 D ABLATION ANALYSIS DETAILS 1633 1634 D.1 FINAL IMAGE QUALITY ASSESSMENT CRITERION The MLLM judges follow the same scoring pipeline as in Appendix B.5. The criterions followed 1637 are slightly altered and are listed as follows: 1638 • Correct Representation: The diagram must accurately depict the concepts, processes, or 1639 data it intends to illustrate without errors. 1640 1641 • Proper Relationships: Ensure that all relationships and interactions between elements are correctly portrayed. 1642 1643 • Legible Text: If there is any labels, legends, and annotations, then they should be easily 1644 readable. Long labels and annotations should be avoided. 1645 Simplicity: The diagram should present information in a straightforward manner, avoiding 1646 unnecessary details that could distract or confuse the learner. 1647 No Redundancy: Ensures that each element serves a purpose without redundant information that could clutter the diagram. 1649 D.2 DETAILED VIEW OF METRICS 1651 This section provides a detailed view of metric used for analysis. 1653 1654 **Yield Rate** This rate calculates percentage of image that are retained at the end of the pipeline. 1655 Specifically, it is 1656 1657 Number of image that compiles successfully and passed through deduplication 1658 Number of generated image 1659 1660 **Compile Success Rate** This rate calculates the compilation success rate 1661 1662 Number of image that compiles successfully Number of generated image **CLIP Score** This score computes the cosine similarity between two image embedding. Specifi-1666 cally, given two images I_1, I_2 , and an image embedding model F, the score is calculated as 1667 1668 $\frac{F(I_1) \cdot F(I_2)}{\|F(I_1)\| \|F(I_2)\|}$ 1670 1671 **CrystalBLEU** A BLEU Papineni et al. (2002) variant and an n-gram-based metric designed to 1672 measure textual similarity. The common n-gram is selected to be the substance code fed into FEYN-1673 MAN as shot example.

1674 D.3 IMAGE AND SUBSTANCE GENERATION ANALYSIS

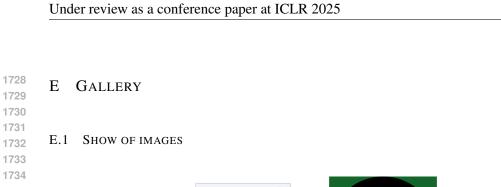
In this section, we hope to provide additional insights into the knowledge and visual diversity of thegenerated diagrams. Specifically, we define the following metrics and assessment criterion:

- *Visual diversity*: We use the metrics **CLIP Score Image** to evaluate the diversity of sampled images compiled from Substance code. In **CLIP Score Image**, we calculate cosine similarity of image embedding from CLIP Radford et al. (2021).
- *Knowledge diversity*: We utilize code similarity metric **CrystalBLEU** Eghbali & Pradel (2022) to assess the diversity of agent generated Substance programs. Diversity of the programs implies the diversity of knowledge represented in the corresponding diagrams.

Category	Setup	Score
	Same Substance	0.9595
Image	Varied Substance	0.8710
	Varied Domain	0.6227
Code	Same Domain	0.0763
Code	Varied Domain	0.0304

Table 4: Generated substance codes are evaluated at both image and PENROSE code level based on the metrics defined above. For images, the lower the score (CLIP score), the more diverse they are. For codes, the lower the score (CrystalBLEU), the more diverse they are. We provide details for both metrics in Appendix D.2

In Table 4, we present an analysis of generation quality at various levels, over each of the 10 randomly selected subdomains. Specifically for images, we assess quality across three tiers. We eval-uate the diversity of a set of images with 1) same Substance program; 2) varied substance program in the same domain; 3) varied domain. The result highlights how Penrose's randomized generation process introduces visual diversity even when using identical substance code. Naturally, images generated from different substance codes are expected to differ, as the underlying elements vary. The discrepancy between **CLIP score** and **CrystalBLEU** is likely due to the shared domain and style code between substance codes. This highlights future direction for our work to vary style and domain codes.



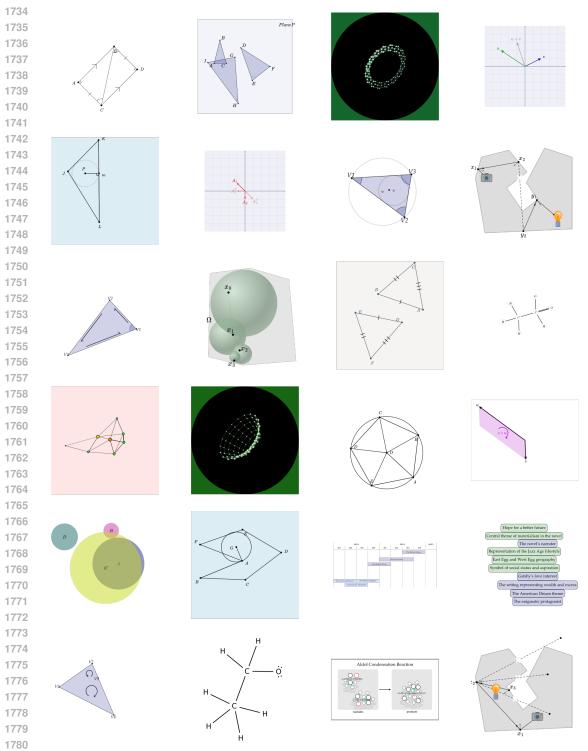
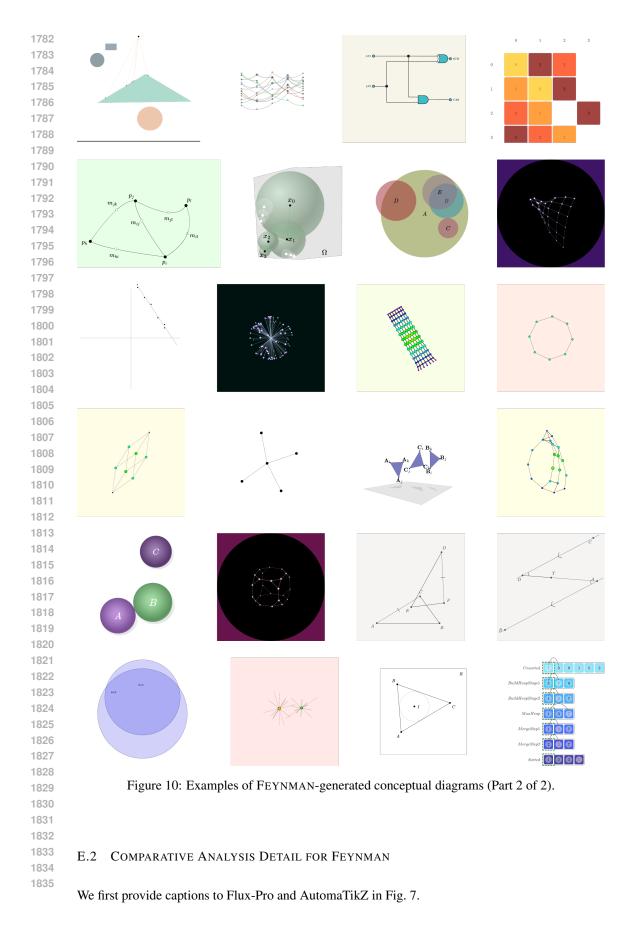


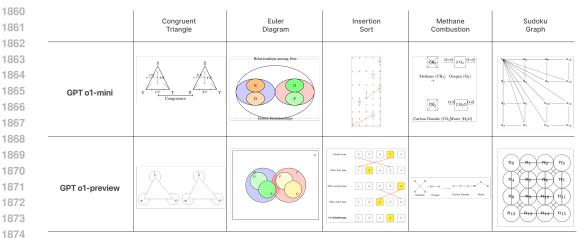


Figure 9: Examples of FEYNMAN-generated conceptual diagrams (Part 1 of 2).



- Insertion Sort: A step-by-step visualization of the insertion sort algorithm applied to the array [5, 3, 8, 1, 4], highlighting the elements being compared and swapped at each stage, ultimately resulting in a sorted array [1, 3, 4, 5, 8].
 - Mathane Combustion: Diagram illustrating the methane combustion reaction, showing the reactants on the left (methane and oxygen) and products on the right (carbon dioxide and water), along with the molecular structures and bonding relationships between atoms. The formula of reaction is: CH4 + 2 02 -> C02 + 2 H2
 - Sudoku Graph: A diagram representing a 4x4 Sudoku graph with 16 nodes labeled from n0 to n15, interconnected by edges that illustrate the relationships between the nodes based on Sudoku rules.
 - **Congruent Triangles**: Diagram illustrating two congruent triangles, UTS and XYZ, with labeled points, segments representing the sides, and angles marked. Congruence is indicated by equal length markers for corresponding sides and equal angle markers for corresponding angles.
 - Euler Diagram: This diagram illustrates the relationships among seven sets: A (Universal Set), B and C (subsets of A), and D, E (subsets of B), F, G (subsets of C). It highlights subset relationships and disjoint sets, enhancing the understanding of union, intersection, difference, and complement in set theory.

1858 We also provide an illustration of drawing TikZ diagram using GPT-o1-preview and GPT-o-mini 1859 below.



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Figure 11: TikZ generation using GPT-40-MINI and GPT-01-PREVIEW

In Fig. 11, we find notable performance using the latest GPT families to generate TikZ code, especially using GPT-o1-preview. Most images were correctly produced within 3 trials, and the quality could be further improved when error message and suggestion are given to the model through multiturn conversation. However, we still find one major drawback of this pipeline compare to FEYN-MAN: TikZ code, once generated, can not be varied in terms of layout. While one way to obtain layout diversity is through multi-turn conversation with the model, there is no constraint to assure the new TikZ code will preserve the original knowledge representation and elements.

5 F REPRODUCIBILITY STATEMENT

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All open-sourced models in Table 2 are evaluated on nodes of NVIDIA RTX A6000 GPUs each with 49 GiB RAM. The detailed evaluation prompt and set up are provided in Appendix C. For our FEYNMAN agent, its hyperparameter and default configuration is provided in Appendix B. We will release DIAGRAMMA and FEYNMAN at the start of review session.