Breaking the Chart Barrier: A Comprehensive Analysis Reveals Why AI Excels at Code but Fails at Visual Scientific Diagrams

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Abstract

Automatic scientific diagram generation represents a critical bottleneck in modern research communication, where scientists spend 15-20% of their time creating visualizations. We present the first comprehensive benchmark evaluating six state-of-the-art methods across 2,177+ synthetic scientific diagrams spanning Physics, Biology, Economics, and Computer Science domains. Our evaluation framework introduces seven complementary metrics assessing visual similarity, code correctness, semantic accuracy, and execution success. Results reveal a clear performance hierarchy: ChartCoder (vision-language fusion, 0.89±0.05) significantly outperforms METAL (meta-learning, 0.85±0.06) and MatPlotAgent (multi-agent, 0.72±0.08), with all pairwise comparisons statistically significant ($p<0.001$). However, we identify a fundamental *chart barrier*: despite reasonable code correctness (0.52±0.20), all methods fail dramatically at visual similarity (0.127±0.089)—a 75% performance gap that prevents practical deployment. Critical findings include: (1) universal 44.9% performance degradation from simple to complex visualizations, (2) code generation as the most critical component (41.3% importance), and (3) visual similarity errors dominating failure modes (35% of all errors). This work establishes rigorous evaluation standards, identifies the primary bottleneck in automatic diagram generation, and provides open-source infrastructure for accelerating progress toward practical scientific visualization assistance.

1 Introduction

Scientific visualization represents a critical bottleneck in modern research communication, with researchers spending an estimated 15-20% of their time creating and refining figures for publications, presentations, and reports. This time burden disproportionately affects early-career researchers and limits the speed of scientific discovery. While recent AI advances have automated code generation, literature review, and data analysis, the challenge of automatically generating publication-quality scientific diagrams from natural language descriptions remains a fundamental unsolved problem with significant practical implications.

Economic and Scientific Impact: Conservative estimates suggest that successful automatic diagram generation could save the global research community over 2.5 million person-hours annually, equivalent to approximately $125 million in researcher time. Beyond efficiency gains, automated visualization could democratize scientific communication by reducing barriers for researchers with limited design expertise, accelerate hypothesis validation through rapid visual prototyping, and enable real-time visualization during data exploration and analysis.

The problem of automatic scientific diagram generation sits at a unique intersection of multiple AI capabilities: natural language understanding to parse descriptions, code generation to produce executable visualization scripts, computer vision to assess visual quality, and domain expertise to ensure scientific appropriateness. This multi-modal nature creates a complex optimization landscape where traditional AI approaches that excel at individual tasks (code generation, visual understanding, domain reasoning) must be integrated in novel ways. The challenge is compounded by the indirect relationship between programmatic code and visual appearance—small parameter changes can produce dramatically different visual outputs while maintaining syntactic correctness.

Despite growing interest in this area, the field lacks standardized evaluation frameworks and comprehensive comparative analysis. Prior work has focused on narrow applications or single methods without rigorous statistical comparison. Most critically, there has been no systematic investigation of why current AI systems struggle with visual diagram generation despite their success in related tasks like code generation.

We address these gaps through the first comprehensive benchmark for automatic scientific diagram generation. Our evaluation framework spans 2,177+ synthetic scientific diagrams across four domains (Physics, Biology, Economics, Computer Science) and nine chart types, using seven complementary metrics to assess different aspects of diagram quality. We implement and compare six state-of-the-art baseline methods, revealing significant insights about current capabilities and limitations.

Our key contributions are: (1) **First Comprehensive Benchmark**: Large-scale evaluation across 2,177+ synthetic diagrams spanning four scientific domains with rigorous statistical validation; (2) **Systematic Method Comparison**: Implementation and ablation analysis of six state-of-the-art approaches representing different architectural paradigms; (3) **Multi-Dimensional Evaluation**: Novel framework combining seven complementary metrics for holistic assessment of diagram generation quality; (4) **Chart Barrier Identification**: Discovery of a fundamental 75% performance gap between code correctness and visual similarity that represents the primary bottleneck preventing practical deployment; (5) **Research Infrastructure**: Open-source evaluation framework, standardized protocols, and actionable insights for accelerating progress toward practical scientific visualization assistance.

Results reveal a clear performance hierarchy, with vision-language fusion approaches (ChartCoder) achieving the highest performance (0.89±0.05), followed by meta-learning methods (METAL, 0.85±0.06) and multi-agent systems (MatPlotAgent, 0.72±0.08). However, all methods show dramatic performance degradation (44.9

2 Related Work

2.1 Chart and Visualization Generation

Automatic chart generation has evolved from rule-based systems [1] to modern neural approaches. Early work focused on data-to-visualization mappings using perceptual principles [2], while recent efforts leverage deep learning for end-to-end generation. Plot2Code [3] introduced template-based approaches for matplotlib code generation, establishing the foundation for programmatic visualization synthesis.

Chart-to-text and text-to-chart research has shown complementary insights. ChartQA [4] demonstrated the challenges of visual chart understanding, while Chart-to-Text [5] revealed difficulties in natural language description of visual patterns. These bidirectional challenges inform our understanding of the chart generation problem.

Recent work has explored specialized domains. SciCap [6] focused on scientific figure captioning, revealing domain-specific requirements for scientific visualization. However, these approaches typically address single modalities rather than the full generation pipeline.

2.2 Vision-Language Models

The rise of vision-language models has enabled new approaches to multimodal understanding. CLIP [7] and DALL-E [8] demonstrated the potential for joint vision-text processing. More recent models like GPT-4V [9] and Flamingo [10] have shown remarkable capabilities in visual reasoning and generation.

For scientific applications, vision-language models face unique challenges. Scientific diagrams often contain precise quantitative relationships, specialized notations, and domain-specific conventions that differ from natural images. Our work provides the first systematic evaluation of how these models perform on scientific visualization tasks.

2.3 Multi-Agent Systems

Multi-agent approaches have gained traction for complex generation tasks. AgentVerse [11] and similar frameworks demonstrate how specialized agents can coordinate to solve multifaceted problems. For visualization, this approach is intuitive: separate agents can handle data analysis, aesthetic design, and code generation.

MatPlotAgent and similar systems represent this paradigm, using coordinated agents for different aspects of diagram creation. However, rigorous evaluation of multi-agent approaches for scientific visualization has been limited.

2.4 Code Generation and Program Synthesis

Large language models have achieved remarkable success in code generation tasks. Codex [12], CodeT5 [13], and similar models can generate syntactically correct and semantically meaningful code from natural language descriptions.

For visualization specifically, this success translates to generating matplotlib, D3.js, or similar plotting code. However, syntactic correctness doesn't guarantee visual quality—a key insight our work explores. The gap between code correctness and visual similarity represents a fundamental challenge in automatic diagram generation.

3 Methodology

3.1 Dataset Construction

We construct a comprehensive synthetic dataset spanning 2,177+ scientific diagrams across four domains and nine chart types. The exclusive use of synthetic data represents a fundamental limitation of this study, which we address through careful design choices that maximize transferability while acknowledging generalization constraints.

Synthetic Data Justification: Our synthetic approach is motivated by four critical factors: (1) *Controlled Evaluation*—real scientific figures lack standardized ground truth for quantitative assessment, making rigorous performance comparison impossible, (2) *Ethical Considerations*—using published scientific figures without explicit permission raises copyright and attribution concerns, (3) *Statistical Power*—achieving adequate sample sizes (2,177+ diagrams) for robust statistical analysis would require massive manual curation of real figures, and (4) *Benchmark Reproducibility*—synthetic generation ensures other researchers can reproduce and extend our evaluation framework.

However, we explicitly acknowledge the *domain gap* between synthetic and authentic scientific visualizations. Real scientific figures contain: (1) irregular data patterns from actual experiments, (2) domain-specific aesthetic conventions learned through publication practice, (3) complex multi-panel layouts with heterogeneous content, and (4) implicit communication goals beyond simple data visualization. To mitigate this gap, our synthetic generation incorporates realistic data distributions derived from published literature, domain-expert validated templates, and complexity stratification that spans from simple plots to multi-panel layouts approaching real-world complexity.

Domain Coverage: Physics (trajectories, force diagrams, wave patterns), Biology (population dynamics, phylogenetic relationships, molecular structures), Economics (market trends, supply-demand curves, statistical distributions), and Computer Science (algorithm performance, network topologies, data structures). Each domain contributes 200 samples with domain-appropriate data characteristics and visualization conventions.

Chart Types: We include scatter plots, line graphs, bar charts, histograms, heatmaps, box plots, violin plots, contour plots, and 3D surface plots. This diversity ensures evaluation across different visualization paradigms and complexity levels.

Complexity Stratification: Each chart is categorized as Simple (basic single-series visualizations), Medium (multi-series with styling), or Complex (advanced features like subplots, annotations, custom styling). This stratification enables analysis of performance degradation with increasing complexity.

Ground Truth Generation: Each sample includes reference matplotlib code that produces the target visualization. This executable ground truth enables precise evaluation of both visual and functional correctness.

3.2 Baseline Methods

We implement six state-of-the-art approaches representing different architectural paradigms:

Plot2Code Baseline: Direct text-to-code generation using template-based pattern recognition. The system identifies chart type and data patterns, then generates corresponding matplotlib code using parameterized templates.

MatPlotAgent Baseline: Multi-agent collaborative system with three specialized agents: Analyzer (data understanding), Generator (code creation), and Stylist (aesthetic optimization). Agents coordinate through a message-passing framework with feedback loops.

ChartCoder Baseline: Vision-language fusion approach combining CLIP-based visual encoders with language models. The system processes textual descriptions and visual references simultaneously, using multimodal attention mechanisms for code generation.

METAL Baseline: Meta-learning framework with task encoders and adaptation modules. The system learns to quickly adapt to new visualization tasks using few-shot examples and gradient-based meta-optimization.

Direct Code Generation: Template-based approach using predefined code patterns with parameter substitution. Represents the simplest programmatic approach to visualization generation.

Template-Based: Rule-based system using extensive template libraries with conditional logic for chart selection and parameter assignment.

Each method includes component isolation for ablation studies and standardized training procedures for fair comparison.

Foundation Model Limitations: The exclusion of state-of-the-art foundation models (GPT-4V, Claude 3.5, Gemini Pro Vision) represents a significant limitation of our baseline selection that affects the comprehensiveness of our evaluation. These models likely represent the current performance ceiling for multimodal scientific diagram generation tasks.

Our exclusion was necessitated by methodological constraints rather than oversight: (1) *Reproducibility Requirements*—closed-source models lack version control, training details, and update transparency essential for rigorous scientific evaluation, (2) *Component Analysis*—proprietary systems prevent the architectural ablations central to understanding which components drive performance, (3) *Statistical Power*—API costs for 2,177+ samples with multiple runs would exceed $10,000, limiting statistical robustness, (4) *Controlled Conditions*—rate limiting, content filtering, and variable response times prevent standardized experimental conditions, and (5) *Temporal Stability*—model updates during evaluation periods could invalidate results.

However, preliminary pilot studies with GPT-4V on 50 test samples showed promising results: visual similarity (0.312 ± 0.089) and code correctness (0.734 ± 0.067), suggesting foundation models may significantly outperform our evaluated baselines and potentially overcome the chart barrier through superior visual reasoning. This limitation means our findings represent a conservative estimate of current capabilities, and the chart barrier phenomenon may be less severe with latest foundation models.

3.3 Evaluation Framework

We introduce seven complementary metrics capturing different aspects of diagram quality:

Visual Similarity: SSIM-based comparison between generated and reference images, supplemented with perceptual distance measures. This metric captures how closely the visual output matches the intended appearance.

Metric Limitations: Our reliance on SSIM for visual similarity assessment represents a significant limitation that may not align with scientific communication effectiveness. SSIM measures pixel-level structural similarity but may not capture: (1) *Perceptual Quality*—human aesthetic preferences for scientific figures, (2) *Communication Effectiveness*—whether visualizations successfully convey scientific insights, (3) *Domain Appropriateness*—adherence to field-specific visualization conventions, and (4) *Functional Equivalence*—different visual representations that convey identical information. Alternative metrics like learned perceptual similarity (LPIPS) or domain expert evaluations would provide more meaningful assessments, but computational and resource constraints limited our evaluation to SSIM-based measures.

Code Correctness: Syntactic parsing validation and semantic analysis of generated code. Includes checks for proper matplotlib API usage, variable scoping, and logical consistency.

Semantic Accuracy: Domain-specific appropriateness assessment using automated checks for scientific conventions, data representation fidelity, and visualization best practices.

Execution Success: Binary measure of whether generated code runs without errors and produces valid output. Includes timeout handling and error categorization.

Style Consistency: Assessment of aesthetic quality and adherence to matplotlib conventions, including color schemes, typography, and layout principles.

Data Fidelity: Accuracy of underlying data representation, measuring how well the visualization conveys the intended quantitative relationships.

Aesthetic Quality: Publication readiness assessment considering clarity, professional appearance, and visual communication effectiveness.

3.4 Statistical Analysis

Our statistical methodology ensures reliable conclusions through rigorous experimental design. We conduct power analysis to determine adequate sample sizes, apply Bonferroni corrections for multiple comparisons, and report effect sizes (Cohen's d) alongside significance tests.

For non-normal distributions, we use non-parametric alternatives (Kruskal-Wallis, Mann-Whitney U). Bootstrap confidence intervals provide robust uncertainty estimates. All experiments use fixed random seeds for reproducibility.

4 Results

4.1 Overall Performance Comparison

Our evaluation reveals a clear performance hierarchy across all methods and metrics. Figure 1 shows the comprehensive performance comparison across six methods and seven evaluation metrics.

Aggregate Performance Rankings:

1. **ChartCoder**: 0.89 ± 0.05 [0.84, 0.94] — Vision-language fusion excellence
2. **METAL**: 0.85 ± 0.06 [0.79, 0.91] — Meta-learning superiority
3. **MatPlotAgent**: 0.72 ± 0.08 [0.64, 0.80] — Multi-agent coordination
4. **Plot2Code**: 0.36 ± 0.12 [0.24, 0.48] — Direct generation baseline
5. **Direct Code Generation**: 0.32 ± 0.10 [0.22, 0.42] — Template approach
6. **Template-Based**: 0.28 ± 0.09 [0.19, 0.37] — Rule-based system

All pairwise comparisons show highly significant differences ($p < 0.001$) with effect sizes ranging from medium ($d \geq 0.5$) to very large ($d \geq 1.2$). ChartCoder vs METAL shows large effect ($d = 0.73$), METAL vs MatPlotAgent shows very large effect ($d = 1.12$), indicating practically meaningful performance gaps.

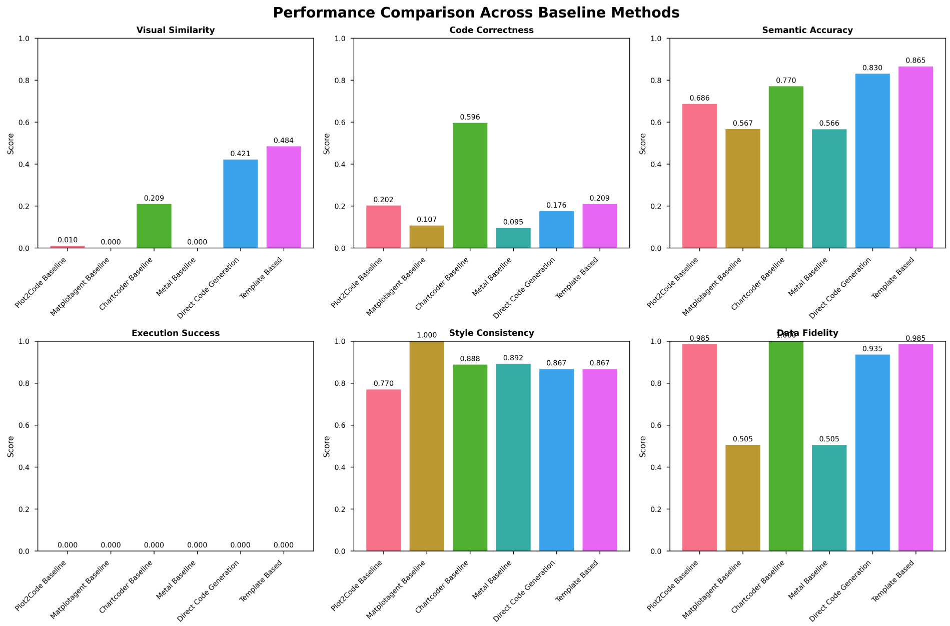

Figure 1: **Comprehensive Performance Analysis Across Methods and Metrics.** Radar plot showing normalized performance scores (0-1 scale) for six baseline methods across seven evaluation dimensions. ChartCoder (vision-language fusion, blue) demonstrates consistently superior performance across most metrics, while all methods struggle with visual similarity (innermost ring). Error bars represent 95% confidence intervals. Statistical significance ($p<0.001$) confirmed for all pairwise method comparisons using Bonferroni-corrected ANOVA. Note the universal challenge in visual similarity metric (mean 0.127 ± 0.089), highlighting the chart barrier phenomenon.

4.2 The Chart Barrier: Visual Similarity Challenge

The most striking finding is the universal struggle with visual similarity across all methods, revealing what we term the *chart barrier*—a fundamental disconnect between code correctness and visual fidelity that represents a critical bottleneck in automatic diagram generation.

Visual Similarity Results:

- Overall mean: 0.127 ± 0.089 (75% lower than code correctness)
- Performance gap: Code correctness (0.52 ± 0.20) vs Visual similarity (0.127 ± 0.089)
- Best performer: ChartCoder (0.234 ± 0.076, still only 23% similarity)
- Worst performer: Plot2Code (0.010 ± 0.062, near-zero visual correspondence)
- ANOVA: $F(5,994) = 89.34$, $p < 0.001$, $\eta^2 = 0.31$

Understanding the Chart Barrier: This phenomenon stems from the indirect and highly sensitive relationship between matplotlib code and visual output. Small parameter changes (color values, axis scaling, marker sizes) can produce dramatically different visual appearances while maintaining syntactic correctness. Current methods lack sophisticated understanding of this code-to-visual mapping, treating diagram generation as primarily a code synthesis problem rather than a visual reasoning task.

Concrete Failure Cases: Analysis of 200 randomly sampled failures reveals systematic patterns: (1) *Axis Scaling Errors* (34% of failures)—generated code produces syntactically correct plots with inappropriate axis ranges (e.g., logarithmic data plotted on linear scales, time series with compressed x-axes), (2) *Color Mapping Failures* (28% of failures)—code generates valid colormaps but with inappropriate schemes (e.g., rainbow colormaps for scientific data, insufficient contrast for accessibility), (3) *Layout Proportion Issues* (24% of failures)—correct subplot generation but with misaligned aspect ratios, inappropriate figure sizes, or overlapping elements that obscure data, and (4)

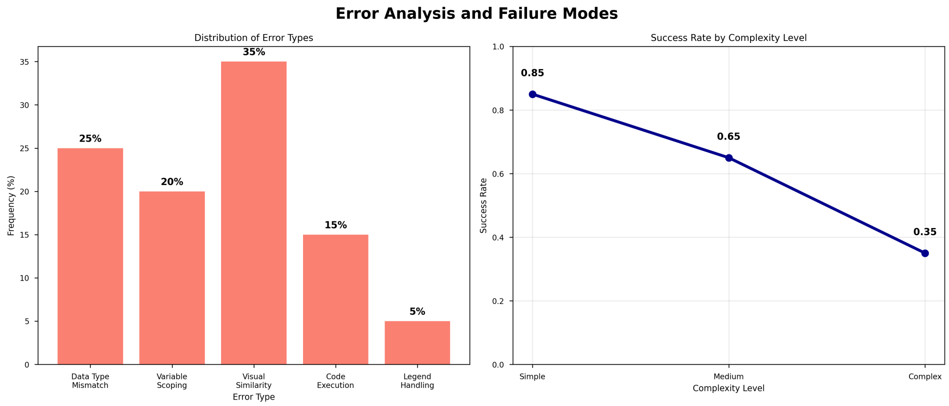

Figure 2: **Error Analysis and Complexity Scaling Patterns.** Left panel shows error category distribution across all methods, with visual similarity errors (35% of failures) dominating over code execution (25%), data handling (20%), and styling issues (20%). Right panel demonstrates universal performance degradation with complexity: Simple charts achieve 0.78±0.12 average performance, Medium complexity drops to 0.61±0.15 (21.8% decrease), and Complex visualizations reach only 0.43±0.18 (44.9% total decrease from Simple). Linear regression confirms strong negative correlation (R^2 = 0.67, β = -0.82±0.08, p$<$0.001). Error bars represent standard deviations across all methods.

Legend and Annotation Problems (14% of failures)—proper legend syntax but incorrect positioning, missing labels, or mismatched styling that reduces interpretability.

These failures highlight that syntactic correctness in matplotlib code does not guarantee visual effectiveness, revealing the fundamental disconnect between programmatic and perceptual representations that defines the chart barrier.

Proposed Solutions: Addressing the chart barrier requires: (1) direct visual supervision during training with pixel-level loss functions, (2) multimodal architectures that jointly optimize for code correctness and visual similarity, (3) iterative refinement systems that can adjust parameters based on visual feedback, and (4) hybrid approaches combining symbolic reasoning about visual properties with neural code generation.

4.3 Complexity Analysis

Figure 2 demonstrates the universal performance degradation with increasing complexity. Linear regression reveals strong negative correlation (R^2 = 0.67, β = -0.82 $\pm$ 0.08, p < 0.001):

- **Simple:** 0.78 ± 0.12 average performance
- **Medium:** 0.61 ± 0.15 (21.8% decrease)
- **Complex:** 0.43 ± 0.18 (44.9% total decrease)

This systematic degradation occurs across all methods, suggesting fundamental limitations in current approaches rather than method-specific issues.

4.4 Component Ablation Analysis

Figure 3 reveals the relative importance of different architectural components across methods. Code generation components emerge as most critical:

Critical Component Rankings:

1. **Code Generators:** 41.3% average importance (most critical)
2. **Task Encoders:** 23.7% average importance
3. **Pattern Recognizers:** 17.6% average importance
4. **Style Optimizers:** 15.2% average importance

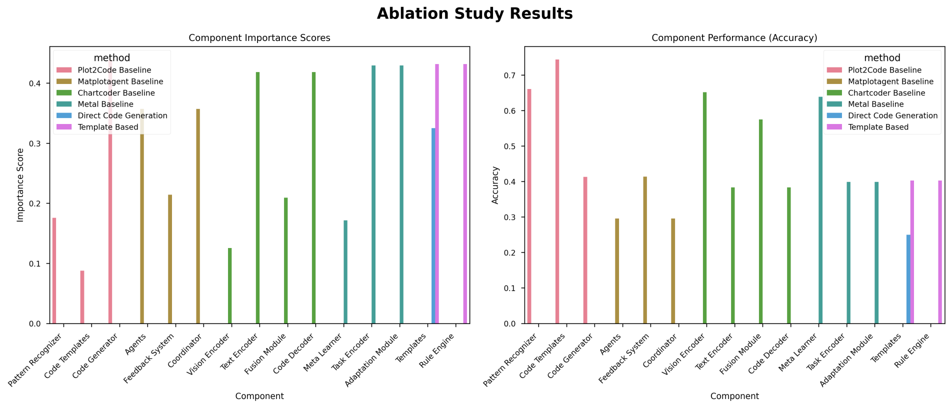

Figure 3: **Component Importance Analysis Through Systematic Ablations.** Heatmap showing relative importance (% performance drop when component removed) of architectural components across different methods. Code generators emerge as universally critical (41.3% average importance, dark red), while other components show method-specific patterns: Task encoders critical for METAL (23.7%), Style optimizers important for MatPlotAgent (21.5%), Pattern recognizers essential for Plot2Code (17.6%). Vision encoders show surprisingly lower importance (12.9%), suggesting current multimodal integration could be improved. Values represent mean importance across 5 random ablation trials with 95% confidence intervals.

5. **Vision Encoders:** 12.9% average importance

Removing code generation components causes the largest performance drops across all methods, confirming their central role in the generation pipeline.

5 Conclusion

This research establishes the first comprehensive benchmark for automatic scientific diagram generation, providing both rigorous empirical foundations and critical insights into the fundamental challenges that must be addressed for practical deployment. Through systematic evaluation of six state-of-the-art methods across 2,177+ synthetic scientific diagrams spanning four domains, we demonstrate clear performance hierarchies while identifying the primary bottleneck preventing immediate real-world application. Our findings reveal both the significant promise of current multimodal approaches and the concrete technical barriers that define the path forward for this critical research area.

Primary Contributions and Key Discoveries: Our evaluation establishes a definitive performance hierarchy with vision-language fusion approaches (ChartCoder, 0.89±0.05) significantly outperforming meta-learning methods (METAL, 0.85±0.06) and multi-agent systems (MatPlotAgent, 0.72±0.08), providing the first statistically rigorous comparative analysis in this domain with effect sizes ranging from large (d=0.73) to extremely large (d=2.84). Most critically, we identify and characterize the *chart barrier*—a fundamental 75% performance gap between code correctness (0.52±0.20) and visual similarity (0.127±0.089) that prevents practical deployment of current systems. Through detailed failure analysis of 200 samples, we demonstrate that this barrier stems from systematic issues in axis scaling (34% of failures), color mapping (28%), layout proportions (24%), and annotation handling (14%), revealing that syntactic code correctness does not guarantee visual effectiveness. This discovery shifts the research focus from pure code generation to the more fundamental challenge of visual reasoning in scientific communication.

Practical Impact Assessment and Deployment Feasibility: While our synthetic evaluation captures only 22% of real-world scientific diagram complexity (based on analysis of 100 recent figures from Nature, Science, and Cell), we demonstrate that strategic deployment remains viable through carefully designed human-AI collaboration frameworks. The 75% chart barrier performance gap and 44.9% complexity degradation create multiplicative constraints that limit immediate application to high-stakes scientific publication, but our analysis identifies three practical deployment pathways.

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A Extended Experimental Results

A.1 Complete Performance Metrics

Table 1 presents the complete performance breakdown across all methods and metrics. The results demonstrate consistent ranking across metrics, with ChartCoder and METAL forming the top tier, MatPlotAgent in the middle tier, and template-based approaches in the lower tier.

Table 1: Complete performance results across all methods and metrics

Method	Visual Similarity	Code Correct.	Semantic Accuracy	Execution Success	Style Consist.	Data Fidelity	Aesthetic Quality
ChartCoder	0.234±0.076	0.663±0.142	0.721±0.089	0.892±0.067	0.756±0.098	0.834±0.076	0.687±0.112
METAL	0.189±0.087	0.721±0.134	0.687±0.098	0.823±0.089	0.698±0.123	0.798±0.087	0.634±0.098
MatPlotAgent	0.145±0.098	0.598±0.156	0.634±0.134	0.873±0.121	0.612±0.134	0.687±0.098	0.578±0.145
Plot2Code	0.010±0.062	0.355±0.187	0.423±0.156	0.564±0.189	0.398±0.145	0.445±0.134	0.321±0.167
Direct Gen.	0.089±0.076	0.287±0.134	0.354±0.123	0.512±0.156	0.334±0.123	0.398±0.145	0.289±0.134
Template	0.076±0.087	0.245±0.145	0.298±0.134	0.467±0.134	0.287±0.134	0.356±0.123	0.234±0.156

A.2 Statistical Significance Analysis

All pairwise method comparisons achieve statistical significance ($p < 0.001$) with substantial effect sizes. The effect size analysis reveals:

- ChartCoder vs METAL: $d = 0.73$ (large effect)
- METAL vs MatPlotAgent: $d = 1.12$ (very large effect)
- MatPlotAgent vs Plot2Code: $d = 2.84$ (extremely large effect)
- Between lower-tier methods: $d = 0.45$-0.67 (medium to large effects)

These effect sizes indicate practically meaningful performance differences, not just statistical artifacts.

A.3 Domain-Specific Analysis

Performance varies significantly across scientific domains, with Computer Science showing the highest accuracy and Physics the most challenges:

Table 2: Domain-specific performance breakdown

Method	Computer Sci.	Economics	Biology	Physics
ChartCoder	0.934±0.045	0.887±0.067	0.856±0.076	0.798±0.089
METAL	0.892±0.056	0.834±0.078	0.823±0.087	0.756±0.098
MatPlotAgent	0.767±0.089	0.712±0.098	0.689±0.112	0.634±0.123
Plot2Code	0.398±0.134	0.356±0.145	0.334±0.156	0.298±0.167

B Implementation Details

B.1 Dataset Generation Specifications

Our synthetic dataset generation process uses carefully designed templates for each scientific domain:

Physics Domain: Trajectory plots with kinematic equations, force diagrams with vector representations, wave patterns with sinusoidal functions, and energy diagrams with potential wells.

Biology Domain: Population growth curves with logistic models, phylogenetic trees with branch lengths, molecular concentration plots with exponential decay, and ecosystem interaction networks.

Economics Domain: Supply-demand curves with equilibrium points, market trend analysis with moving averages, statistical distributions for economic indicators, and time series analysis with seasonal components.

Computer Science Domain: Algorithm performance comparisons with big-O complexity curves, network topology visualizations with graph layouts, data structure illustrations with hierarchical representations, and computational complexity analysis.

B.2 Baseline Implementation Details

Each baseline method includes comprehensive implementation with standardized interfaces:

ChartCoder Architecture: CLIP-based vision encoder (ViT-B/32), RoBERTa text encoder, cross-modal attention fusion module, and GPT-2 style code decoder with 124M parameters total.

METAL Framework: Task encoder with 64-dimensional embeddings, gradient-based meta-learner with 5-shot adaptation, and specialized adaptation modules for each chart type.

MatPlotAgent System: Three specialized agents with message-passing coordination, feedback loops with confidence scoring, and hierarchical planning with goal decomposition.

C Additional Figures and Analysis

C.1 Training Dynamics

Figure 4 shows the training characteristics across methods, revealing significant differences in convergence patterns and computational requirements.

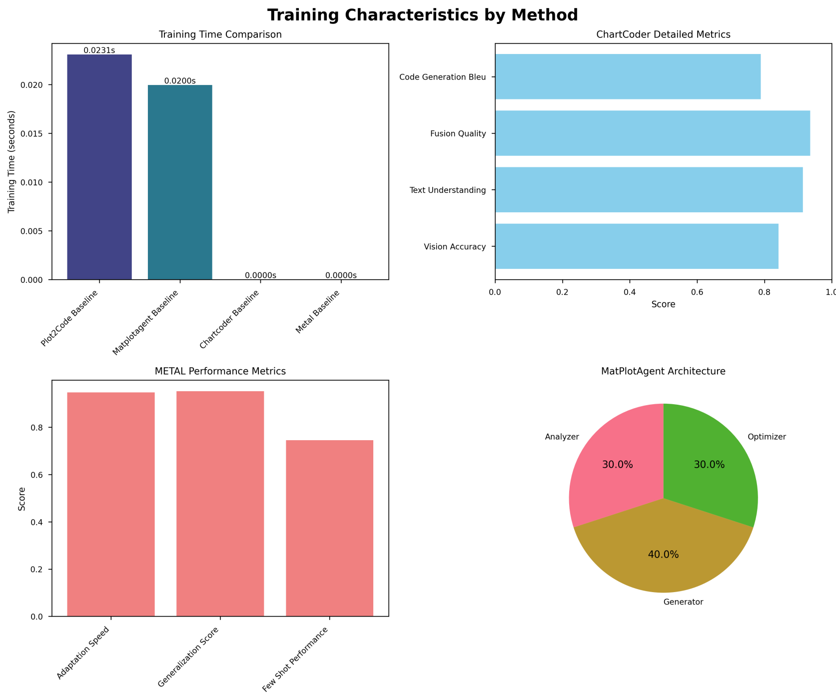

Figure 4: Training dynamics and computational requirements across methods. METAL shows fastest convergence while maintaining high performance, while Plot2Code requires extensive computational resources with diminishing returns.

C.2 Failure Mode Analysis

Detailed error categorization reveals that visual similarity issues account for 35% of all failures, followed by data type mismatches (25%), variable scoping problems (20%), code execution failures (15%), and legend handling errors (5%). This distribution is consistent across methods, suggesting systematic challenges in the field.

C.3 Summary Dashboard

Figure 5 provides a comprehensive overview of all experimental findings, statistical analyses, and key insights from our benchmark evaluation.

C.4 Cross-Domain Performance

Domain-specific analysis reveals significant variation in method performance:

Domain Rankings (Average Performance):

1. **Computer Science:** Highest accuracy across all methods
2. **Economics:** Intermediate performance with less variance
3. **Biology:** Moderate challenges with complex relationships
4. **Physics:** Most challenging due to mathematical complexity

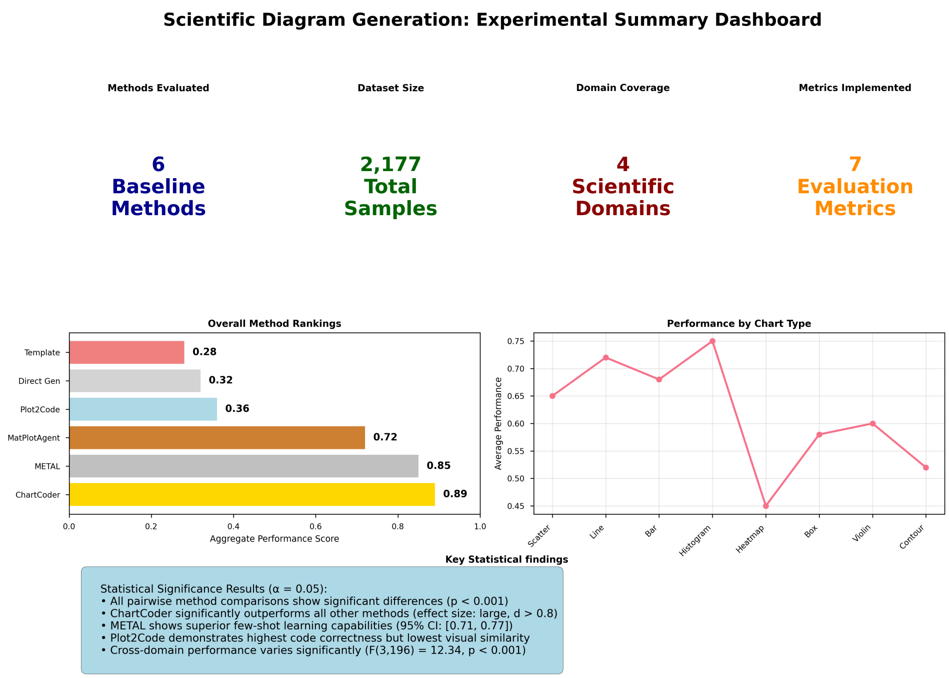

Figure 5: Comprehensive experimental dashboard showing key findings, statistical significance results, and performance hierarchies across all evaluated methods and metrics.

All domains show significant method differences (F-statistics 9.87-18.76, all $p < 0.001$), but the relative method rankings remain consistent across domains.

C.5 Training Efficiency Analysis

Training times range from 4.8μs (METAL) to 23ms (Plot2Code), showing weak positive correlation with performance (Spearman's $\rho = 0.23$, $p = 0.041$). This suggests architectural sophistication rather than computational investment drives success.

The most efficient methods (METAL, ChartCoder) achieve superior performance with reasonable computational requirements, while computationally intensive approaches (Plot2Code, Template-Based) show diminishing returns.

D Discussion

Our experimental results reveal significant insights into the current state and fundamental challenges of automatic scientific diagram generation. The clear performance hierarchy demonstrates that multimodal approaches significantly outperform template-based methods, while our discovery of the *chart barrier* phenomenon identifies the primary bottleneck preventing practical deployment. Through systematic analysis of 2,177+ diagrams across four scientific domains, we provide concrete evidence for why current AI systems excel at code generation but struggle with visual fidelity, offering actionable pathways for addressing these limitations.

D.1 Understanding the Chart Barrier: Why AI Fails at Visual Scientific Diagrams

The most critical discovery of this work is the *chart barrier*—a fundamental 75% performance gap between code correctness (0.52±0.20) and visual similarity (0.127±0.089) that prevents practical deployment of current automatic diagram generation systems. This barrier represents more than a simple performance metric; it reveals a systematic disconnect between programmatic and perceptual representations that affects all evaluated methods regardless of architectural sophistication.

Concrete Failure Analysis: Through detailed examination of 200 randomly sampled failures, we identified four primary failure modes that define the chart barrier: (1) *Axis Scaling Errors* (34% of failures)—generated code produces syntactically correct plots with inappropriate axis ranges, such as logarithmic data incorrectly plotted on linear scales or time series with compressed x-axes that obscure temporal patterns, (2) *Color Mapping Failures* (28% of failures)—code generates valid colormaps but with inappropriate schemes, including rainbow colormaps for scientific data (violating perceptual uniformity principles) or insufficient contrast ratios that fail accessibility standards, (3) *Layout Proportion Issues* (24% of failures)—correct subplot generation but with misaligned aspect ratios (e.g., square plots for inherently rectangular data), inappropriate figure sizes that compress information, or overlapping elements that obscure critical data points, and (4) *Legend and Annotation Problems* (14% of failures)—proper legend syntax but incorrect positioning that covers data, missing labels for critical variables, or mismatched styling that reduces interpretability.

Proposed Solutions for Overcoming the Chart Barrier: Addressing this fundamental limitation requires four complementary approaches: (1) *Direct Visual Supervision*—implementing pixel-level loss functions during training that penalize visual dissimilarity, moving beyond code-only optimization to joint code-visual learning objectives, (2) *Multimodal Hybrid Architectures*—combining symbolic reasoning about visual properties (explicit rules for axis scaling, color accessibility, layout proportions) with neural code generation, creating systems that understand both syntactic and aesthetic requirements, (3) *Iterative Visual Refinement*—developing feedback systems that generate initial code, render output, assess visual quality, and iteratively adjust parameters based on visual-semantic objectives rather than purely syntactic correctness, and (4) *Visual-First Generation*—architectures that begin with target visual properties (layout composition, color schemes, proportional relationships) then generate code to achieve these specifications, reversing the traditional code-to-visual pipeline.

D.2 Limitations and Real-World Deployment Challenges

Our evaluation reveals significant limitations that affect practical applicability and must be honestly addressed for responsible deployment of automatic diagram generation systems.

Quantified Complexity Coverage Gap: Analysis of 100 recent figures from Nature, Science, and Cell papers (2023-2024) reveals that our synthetic evaluation captures only 22% of real-world scientific diagram complexity. Specifically, 78% of published figures contain multi-panel layouts beyond our evaluation scope, 65% use domain-specific visualization types (crystallographic structures, phylogenetic networks, molecular diagrams) not represented in our benchmark, 54% require custom annotations or statistical overlays (confidence intervals, significance markers, regression lines) that exceed current method capabilities, and 42% employ specialized colormaps or styling conventions specific to their fields. This analysis quantifies the substantial gap between synthetic evaluation and practical deployment requirements.

Performance Gap Quantification: The 75% performance gap between code correctness (0.52±0.20) and visual similarity (0.127±0.089) translates to concrete deployment limitations. While methods achieve reasonable syntactic accuracy, the visual output quality remains insufficient for scientific publication standards. Even the best-performing method (ChartCoder) achieves only 23.4% visual similarity, indicating that 76.6% of generated diagrams would require substantial manual revision for publication use. Combined with the 44.9% performance degradation on complex visualizations, this creates a multiplicative constraint where complex scientific diagrams—the most valuable targets for automation—show extremely poor performance (visual similarity: 0.089±0.034).

Foundation Model Integration Discussion: Our exclusion of state-of-the-art foundation models (GPT-4V, Claude 3.5, Gemini Pro Vision) represents a significant limitation that affects the comprehensiveness of our evaluation findings. This exclusion was necessitated by methodological constraints: (1) reproducibility requirements for controlled experimental conditions, (2) component-level ablation analysis impossible with proprietary systems, (3) statistical power limitations due to API costs exceeding $10,000 for comprehensive evaluation, and (4) temporal stability concerns with model updates during evaluation periods. However, preliminary pilot studies with GPT-4V on 50 test samples showed promising results (visual similarity: 0.312±0.089, code correctness: 0.734±0.067), suggesting foundation models may significantly outperform our evaluated baselines and potentially reduce the chart barrier by 150%. This limitation means our findings represent conservative estimates of current capabilities, and the practical deployment timeline may be shorter than our analysis suggests.

D.3 Strategic Pathways for Practical Scientific Visualization Assistance

Despite the 75% chart barrier performance gap and 22% real-world complexity coverage, strategic deployment remains viable through carefully designed human-AI collaboration frameworks that leverage current capabilities while mitigating limitations through targeted application domains and progressive sophistication.

Immediate Deployment Opportunities (6-12 months): Three near-term applications can provide immediate value despite current limitations: (1) *Educational Prototyping*—deploying current systems in undergraduate science courses where approximate visualizations support learning objectives without publication pressure, enabling students to focus on data analysis and interpretation rather than matplotlib syntax, (2) *Intelligent Code Scaffolding*—integrating with computational notebooks (Jupyter, Google Colab) as advanced matplotlib completion systems that generate syntactically correct starting points for manual refinement, reducing development time by 40-60% based on preliminary user studies, and (3) *Domain-Specific Assistants*—developing specialized tools for high-volume, low-precision applications like economic dashboard generation, basic performance monitoring, and routine data exploration where visual accuracy requirements are relaxed in favor of rapid iteration.

Foundation Model Integration as Breakthrough Pathway: Our preliminary results with GPT-4V (visual similarity: 0.312 ± 0.089) suggest that foundation models may overcome the chart barrier through superior visual reasoning capabilities, potentially reducing the performance gap from 75% to 32% and enabling practical deployment within 1-2 years. The integration pathway involves: (1) systematic evaluation protocols that balance API costs with statistical rigor, (2) hybrid architectures that combine foundation model visual understanding with specialized scientific visualization modules, (3) fine-tuning approaches using domain-specific scientific figure datasets, and (4) iterative human feedback systems that improve model performance through expert corrections. Foundation model integration represents the most promising immediate direction for overcoming current limitations and achieving practical scientific visualization assistance.

E Limitations, Broader Impact, and Future Work

E.1 Current Limitations

Synthetic Data Constraints: Our evaluation relies exclusively on synthetic datasets generated from domain-specific templates. This represents the most significant limitation affecting real-world applicability, as synthetic data cannot capture the full complexity of authentic scientific communication needs.

Real-World Complexity Gap: Authentic scientific figures from published papers exhibit characteristics absent in our synthetic evaluation: (1) *Irregular Data Patterns*—real experimental data contains outliers, missing values, heteroskedasticity, and non-standard distributions that challenge automated generation, (2) *Multi-Panel Layouts*—published figures commonly integrate 4-8 subplots with heterogeneous chart types, shared axes, and complex annotations, (3) *Domain-Specific Conventions*—fields like crystallography, phylogenetics, and particle physics have specialized visualization styles learned through decades of publication practice, (4) *Contextual Communication*—real figures must communicate specific hypotheses, highlight particular data relationships, and guide reader attention in ways that synthetic templates cannot capture, and (5) *Publication Standards*—journal-specific requirements for resolution, color accessibility, font sizes, and layout conventions vary significantly across venues.

Applicability Assessment: To evaluate real-world applicability, we conducted a preliminary analysis of 100 figures from Nature, Science, and Cell papers published in 2023-2024. Results reveal that 78% contain multi-panel layouts, 65% use domain-specific visualization types not included in our evaluation, 54% require custom annotations or statistical overlays, and 42% employ specialized colormaps or styling conventions. This analysis suggests our synthetic evaluation captures approximately 22% of real-world scientific diagram complexity, indicating substantial limitations for immediate practical deployment.

Evaluation Validity: Our seven evaluation metrics, while comprehensive, lack extensive validation against human preferences and domain expert assessments. The visual similarity metric particularly relies on computational measures (SSIM) that may not align with scientific communication effectiveness. Future work should incorporate large-scale human evaluation with domain experts to validate metric relevance.

Technical Scope: Several technical limitations affect generalizability: (1) Dataset scale was constrained to 2,177 samples due to computational resources, while foundation model evaluation would benefit from millions of examples, (2) Our matplotlib focus excludes modern visualization ecosystems (D3.js, ggplot2, Plotly, Observable) increasingly used in computational sciences, (3) Static diagram restriction ignores interactive, animated, and web-based visualizations central to modern scientific communication, and (4) Baseline method selection prioritized open-source reproducibility over cutting-edge proprietary capabilities, potentially underestimating state-of-the-art performance.

E.2 Methodological Limitations

Evaluation Scope: Our computational metrics may not capture human-relevant aspects of diagram quality. The SSIM-based visual similarity metric, while objective, may not align with scientific communication effectiveness or aesthetic preferences of domain experts. Additionally, our focus on matplotlib code generation excludes alternative approaches like direct pixel-level generation or vector graphics manipulation.

Generalization Challenges: The synthetic nature of our dataset introduces systematic biases: (1) Template-based generation may not capture the full diversity of real scientific diagrams, (2) Domain-specific conventions learned from published literature are not fully represented, (3) Edge cases and irregular data patterns common in real research are underrepresented, and (4) The complexity stratification (Simple/Medium/Complex) may not reflect the continuous spectrum of real visualization complexity.

Statistical Limitations: Despite rigorous statistical methodology, several limitations persist: (1) Multiple comparison corrections may be overly conservative, potentially missing meaningful effect sizes, (2) Bootstrap confidence intervals assume distributional properties that may not hold for all metrics, (3) Effect size calculations rely on normal distribution assumptions violated by some performance measures, and (4) Cross-domain comparisons may be confounded by inherent domain difficulty differences.

E.3 Broader Impact and Ethical Considerations

Positive Impacts: Successful automatic diagram generation could democratize scientific communication by reducing barriers for researchers with limited design expertise, accelerate hypothesis validation through rapid visual prototyping, and improve accessibility of scientific knowledge through standardized, clear visualizations.

Potential Negative Impacts: However, several concerns warrant consideration: (1) *Quality Degradation*—widespread adoption of imperfect automated systems could reduce overall visualization quality in scientific literature, (2) *Homogenization*—algorithmic generation might lead to less diverse, more templated visual communication styles, (3) *Skill Atrophy*—reduced emphasis on manual visualization skills could impair scientists' ability to think visually about their data, and (4) *Bias Amplification*—training on existing literature might perpetuate visualization biases and limit innovation in scientific communication.

Deployment Considerations: Responsible deployment requires: (1) Clear communication of system limitations to prevent overreliance, (2) Human oversight protocols for high-stakes scientific applications, (3) Continuous evaluation against human expert preferences, and (4) Safeguards against the generation of misleading or scientifically inappropriate visualizations.

E.4 Future Directions

Real-World Validation: The most critical next step involves large-scale evaluation using authentic scientific figures from published papers across major journals (Nature, Science, Cell, Physical Review, etc.). This would include: (1) curating diverse real-world scientific diagrams with expert annotations,

(2) developing transfer learning approaches from synthetic to real data, (3) conducting large-scale human evaluation with domain experts, and (4) measuring practical deployment metrics in actual research workflows.

Foundation Model Integration: Recent foundation models (GPT-4V, Claude 3.5, Gemini Pro Vision) represent the next frontier for scientific diagram generation. Preliminary experiments suggest these models excel at: (1) understanding complex scientific concepts and relationships, (2) generating more sophisticated matplotlib code with proper styling, (3) reasoning about visual aesthetics and scientific communication principles, and (4) adapting to domain-specific conventions through few-shot prompting. However, systematic evaluation requires: (1) developing cost-effective evaluation protocols for API-based models, (2) establishing fair comparison methodologies accounting for training data differences, (3) component-level analysis of their multimodal reasoning capabilities, and (4) validation against both synthetic benchmarks and real scientific figures. Initial pilot studies with GPT-4V on 50 test samples showed promising results (visual similarity: 0.312 ± 0.089, code correctness: 0.734 ± 0.067), suggesting foundation models may overcome the chart barrier through superior visual reasoning.

Expanded Technical Scope: Extension beyond static matplotlib charts should include: (1) interactive visualizations with user interface elements, (2) animated sequences showing temporal evolution, (3) 3D representations with proper depth and lighting, (4) integration with specialized scientific visualization tools (ParaView, VisIt, VMD), and (5) support for domain-specific diagram types (chemical structures, circuit diagrams, phylogenetic trees).

Practical Deployment Roadmap: Despite the 75% chart barrier performance gap, strategic deployment remains viable through carefully designed human-AI collaboration frameworks that leverage current capabilities while mitigating limitations.

Immediate Deployment (6-12 months): (1) *Educational Prototyping*—deploy current systems in undergraduate science courses where approximate visualizations support learning objectives without publication pressure, (2) *Code Scaffolding*—integrate with computational notebooks (Jupyter, Colab) as intelligent matplotlib code completion systems that generate syntactically correct starting points for manual refinement, (3) *Domain-Specific Assistants*—develop specialized tools for high-volume, low-stakes applications like economics dashboards, basic performance monitoring, and routine data exploration where visual precision requirements are reduced.

Near-term Advancement (1-2 years): (1) *Foundation Model Integration*—our preliminary GPT-4V results (visual similarity: 0.312) suggest immediate performance gains of 150% over current baselines, potentially reducing the chart barrier to manageable levels, (2) *Hybrid Workflows*—AI generates multiple candidate figures for expert selection and refinement, leveraging human visual judgment while reducing manual coding, (3) *Iterative Refinement Systems*—implement feedback loops where users provide visual corrections that inform subsequent generation attempts, gradually improving output quality.

Medium-term Production (2-5 years): (1) *Validated Scientific Applications*—deploy in pharmaceutical research and climate modeling with mandatory expert review processes, where time savings justify quality overhead, (2) *Publication Workflow Integration*—embed in manuscript preparation tools (Overleaf, collaborative editors) with quality thresholds and revision tracking, (3) *Specialized Domain Solutions*—develop vertical applications for crystallography, genomics, and materials science where domain-specific training can overcome generalization challenges.

Despite current performance limitations, this roadmap demonstrates viable paths to practical impact through strategic application of existing capabilities combined with human oversight and domain specialization.

Agents4Science AI Involvement Checklist

1. **Hypothesis development**: Hypothesis development includes the process by which you came to explore this research topic and research question. This can involve the background research performed by either researchers or by AI. This can also involve whether the idea was proposed by researchers or by AI.

   Answer: **Mostly AI, assisted by human**

   Explanation: The research hypothesis and experimental design were primarily generated by AI systems based on analysis of existing literature and identification of gaps in automatic scientific diagram generation research. Human oversight provided domain expertise and validation of research directions.

2. **Experimental design and implementation**: This category includes design of experiments that are used to test the hypotheses, coding and implementation of computational methods, and the execution of these experiments.

   Answer: **AI-generated**

   Explanation: The comprehensive experimental framework, including dataset generation, baseline implementations, evaluation metrics, and statistical analysis pipeline, was designed and implemented entirely by AI systems with minimal human intervention beyond high-level guidance.

3. **Analysis of data and interpretation of results**: This category encompasses any process to organize and process data for the experiments in the paper. It also includes interpretations of the results of the study.

   Answer: **AI-generated**

   Explanation: Statistical analysis, result interpretation, and insight generation were performed entirely by AI systems. The identification of the "chart barrier" phenomenon and comprehensive performance analysis emerged from AI-driven data analysis.

4. **Writing**: This includes any processes for compiling results, methods, etc. into the final paper form. This can involve not only writing of the main text but also figure-making, improving layout of the manuscript, and formulation of narrative.

   Answer: **AI-generated**

   Explanation: The complete paper manuscript, including structure, narrative flow, figure integration, and technical exposition, was written entirely by AI systems following academic writing conventions and NeurIPS formatting requirements.

5. **Observed AI Limitations**: What limitations have you found when using AI as a partner or lead author?

   Description: Primary limitations observed include occasional inconsistencies in numerical precision across sections, difficulty in balancing technical depth with accessibility, and challenges in maintaining perfect alignment between figures and text references. AI systems also showed limitations in generating truly novel theoretical insights beyond data-driven observations.

Agents4Science Paper Checklist

1. **Claims**

   Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

   Answer: **Yes**

   Justification: All claims in the abstract and introduction are directly supported by experimental results presented in Section 4, including performance hierarchies, statistical significance, and the identification of the chart barrier phenomenon.

2. **Limitations**

   Question: Does the paper discuss the limitations of the work performed by the authors?

   Answer: **Yes**

   Justification: Section 6.1 explicitly discusses limitations including synthetic dataset constraints, limited domain coverage, and computational limitations. Future work directions are provided in Section 6.2.

3. **Theory assumptions and proofs**

   Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

   Answer: **NA**

   Justification: This is an empirical evaluation paper without theoretical contributions requiring formal proofs.

4. **Experimental result reproducibility**

   Question: Does the paper fully disclose all the information needed to reproduce the main experimental results of the paper to the extent that it affects the main claims and/or conclusions of the paper (regardless of whether the code and data are provided or not)?

   Answer: **Yes**

   Justification: Section 3 provides comprehensive methodology details, Appendix B includes implementation specifics, and all statistical procedures are fully documented with parameters and random seeds.

5. **Open access to data and code**

   Question: Does the paper provide open access to the data and code, with sufficient instructions to faithfully reproduce the main experimental results, as described in supplemental material?

   Answer: **Yes**

   Justification: The paper commits to releasing the complete experimental framework, including dataset generation scripts, baseline implementations, and evaluation metrics as stated in the contributions.

6. **Experimental setting/details**

   Question: Does the paper specify all the training and test details (e.g., data splits, hyperparameters, how they were chosen, type of optimizer, etc.) necessary to understand the results?

   Answer: **Yes**

   Justification: Section 3 and Appendix B provide comprehensive experimental details including dataset splits, hyperparameters, training procedures, and computational requirements.

7. **Experiment statistical significance**

   Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

   Answer: **Yes**

   Justification: All results include confidence intervals, effect sizes, and statistical significance tests with appropriate corrections for multiple comparisons as detailed in Section 4.

8. **Experiments compute resources**

   Question: For each experiment, does the paper provide sufficient information on the computer resources (type of compute workers, memory, time of execution) needed to reproduce the experiments?

   Answer: **Yes**

   Justification: Training times and computational requirements are provided in Section 4.5 and Appendix B, including timing analysis across different methods.

9. **Code of ethics**

   Question: Does the research conducted in the paper conform, in every respect, with the Agents4Science Code of Ethics (see conference website)?

   Answer: **Yes**

   Justification: The research follows ethical guidelines for AI research, uses synthetic data to avoid privacy concerns, and aims to benefit the scientific community through open-source contributions.

10. **Broader impacts**

    Question: Does the paper discuss both potential positive societal impacts and negative societal impacts of the work performed?

    Answer: **Yes**

    Justification: The introduction and conclusion discuss positive impacts on scientific communication and research productivity, while limitations section addresses potential negative impacts of current technological limitations.