Towards Multi-Agent Reasoning Systems for Collaborative Expertise Delegation: An Exploratory Design Study

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Abstract

Designing effective collaboration structure for multi-agent systems to stimulate collective reasoning capability is crucial yet remains underexplored. In this paper, we systematically investigate how collaborative reasoning performance is affected by three key design factors: (1) expertise-domain alignment, (2) collaboration paradigm (structured workflow vs. diversity-driven integration), and (3) system scale. Our findings reveal that expertise alignment benefits are highly domain-contingent, proving most effective for contextual reasoning tasks. Furthermore, collaboration focused on integrating diverse responses consistently outperforms sequential functional cooperation. Finally, we empirically explore the impact of scaling the multi-agent system with expertise specialization and study the computational trade off, highlighting the need for more efficient communication protocol design. Our work provides concrete guidelines for configuring specialized multi-agent system and identifies critical architectural trade-offs and bottlenecks for scalable multi-agent reasoning.

1 Introduction

Collective intelligence, the emergent problem-solving capability arising from structured group interactions, has long been recognized as a cornerstone of complex human decision-making (Surowiecki, 2004). Through mechanisms like deliberative debate and systematic knowledge integration, human collectives consistently outperform individual experts in tasks requiring multi-perspective analysis and contextual synthesis.

The recent evolution of large language and reasoning models (LLMs/LRMs; Yang et al., 2025; Jaech et al., 2024; Team et al., 2025) has spurred parallel investigations into machine collective intelligence. Contemporary research has developed artificial analogs of human collaboration patterns through techniques such as multi-agent debate

Figure 1: Workflow diagram for a multi-agent reasoning system with specialized agents.

frameworks and workflow orchestration (Li et al., 2024c; Du et al., 2024; Liang et al., 2024). These approaches primarily focus on either enhancing individual model performance through collective verification processes or establishing general-purpose problem-solving workflow pipelines.

A prevalent strategy to enhance collective intelligence in these systems is collaborative expertise specialization, where LLMs are instructed to simulate specific expert personas (e.g., "act as an experienced lawyer"; Li et al., 2024a; Xu et al., 2024a). This approach is hypothesize to operate through two primary mechanisms: (1) knowledge recall: activating relevant domain-specific knowledge latent within the LLMs via contextual role framing, and (2) perspective synthesis: leveraging diverse expert viewpoints to foster emergent, robust problem-solving patterns.

Although expertise specialization is widely adopted in multi-agent system (Wang et al., 2024a; Li et al., 2024a), the impact of varying collaborative expertise domain on distinct downstream scenarios remains underexplored, making configuring multiple expert roles unclear in multi-agent study. To address this gap, we empirically evaluate the influence of different collaborative expertise configurations on task performance across four repre-

sentative domains from MMLU-pro (Wang et al., 2024d). **Our findings in Section 4 demonstrate a positive correlation between task performance and the alignment of group expertise with the task domain**, further underscoring the necessity of accurately matching the multi-agent system expertise with downstream tasks.

Another dimension concerning the multi-agent system design is the collaboration paradigm—namely, the mechanism governing how specialist agents interact in a multi-agent system. Currently, the collaboration paradigm predominantly used in recent studies could be categorized into two kinds: (1) Diversity-Driven Perspective Integration, where agents, often embodying different viewpoints or roles, are encouraged to generate diverse responses to enrich the solution space (Wang et al., 2024b; Chen et al., 2024b; Hu et al., 2025). (2) Structured Workflow Cooperation, where different agents are assigned distinct sub-tasks within a predefined pipeline to collaboratively construct a solution (Chen et al., 2024c; Hong et al., 2024; Zhang et al., 2025). To understand the preference of collaboration paradigm in collaborative expertise specialization, we design comparative experiments which unveil the performance differences between paradigms. **Our observations in Section 5 reveal a consistent advantage for diversity-driven collaboration over structured workflow collaboration, suggesting the superiority of the diversity-driven paradigm.** Detailed analysis regarding intra-system viewpoint diversity are also conducted to study the impact of agent response diversity in multi-agent system, where we find a higher diversity could indicate a better performance.

Finally, constructing large-scale multi-agent system has become a critical, yet often enigmatic aspect of multi-agent system design (Chen et al., 2024c; Piao et al., 2025). While intuition and some preliminary studies (Qian et al., 2024; Li et al., 2023) suggest that larger groups would lead to a better reasoning performance, the actual effectiveness of scaling within the context of collaborative expertise specialization and the potential computation-performance trade-off, are not well understood. Motivated by the lack of clarity on scaling effects in collaborative expertise specialization, we specifically study how performance scales in multi-agent systems composed of specialized experts. Our systematic experiments involve incrementally increasing the system scale to examine potential scaling laws. **The results in Section 6 uncover non-linear dynamics; specifically, adding more experts tends to improve the collective reasoning ability of the system. This positive trend holds regardless of whether the larger system scale contains greater viewpoint diversity or a more comprehensive workflow structure**, indicating a general benefit to increasing the number of expert agents and encouraging such designs for enhanced system performance. Furthermore, our analysis of the computational trade-offs associated with system scaling reveals that, while the system would benefit from the expansion, there remains a critical need for more efficient communication protocols between agents for more scalable and cost-effective multi-agent reasoning process.

2 Related Works

2.1 Multi-Agent Collaboration

Multi-Agent Collaboration adopts multiple LLMs to solve the problem collaboratively. Abundant researches have investigated the multi-agent collaboration framework to improve decision-making capability of the system (Wang et al., 2024b; Liang et al., 2024; Du et al., 2024). In addition to collaboration among LLMs, several researchers instruct the agents to cooperate in a workflow to study the multi-agent systems' ability of solving real world challenges (Li et al., 2024b; Xu et al., 2024b; Chen et al., 2024a). While Qian et al. (2024), Yang et al. (2024) and Wang et al. (2024c) has investigate the effect of varying the scale of multi-agent system on reasoning and simulation, prior researches have not systematically examined the interplay between collective expertise specialization, collaboration mechanisms, and the impact of system scale simultaneously. In this work, we conduct extensive experiments to formally analyze the influence of these three critical dimensions on multi-agent collaborative reasoning. Our findings provide actionable insights toward more effective system design.

2.2 LLMs as Domain Experts

The rapid evolution of LLMs has endowed them with vast repositories of domain-specific knowledge, enabling their application across a wide range of expert tasks. Recent researches have explored the potential of LLMs to emulate specific personas by conditioning them on detailed character profiles (Chan et al., 2024; Samuel et al., 2024; Xu et al., 2023). These studies demon-

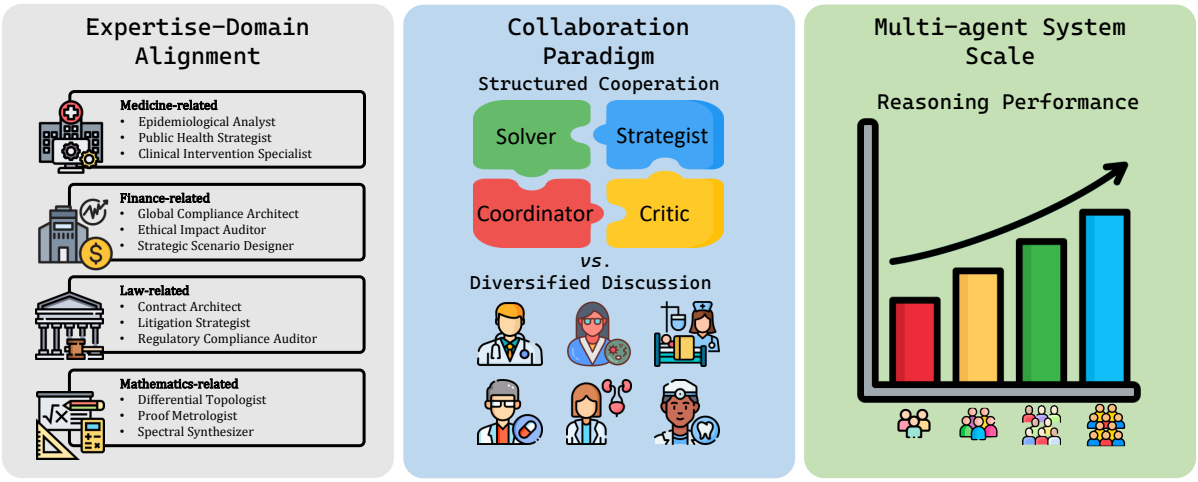

Figure 2: Demonstration of three key factors characterizing research on multi-agent collaborative reasoning systems. (1) expertise-domain alignement, (2) collaboration paradigm, and (3) scale of the multi-agent system.

strate that by providing LLMs with demographic or role-specific prompts, they can effectively exhibit human-like personality traits and behaviors. Furthermore, Kong et al. (2024) and Xu et al. (2023) have shown that instructing LLMs to simulate domain experts can enhance their reasoning capabilities in specialized contexts, underscoring the necessity of introducing expert knowledge into reasoning process. Despite these advancements and the growing prominence of multi-agent systems in research, the specific impact of collaborative expertise specialization on reasoning performance remains underexplored. In this paper, through meticulously designed experiments, we systematically investigate the impact of expertise specialization within multi-agent reasoning systems. Our findings reveal that simulating specialized roles significantly enhances performance on tasks requiring contextual reasoning, while showing limited influence on those primarily dependent on factual recall or mathematical deduction.

3 Preliminary

3.1 Problem Setup

Formally, given a multi-agent system $\mathcal{M}_n = \{\mathcal{A}_1, \mathcal{A}_2, ..., \mathcal{A}_n\}$ where n indicates the number of agents inside the system and $\mathcal{A}_i$ represents the i-th agent of the system, a query $\mathcal{Q}$, and a set of candidate options $\mathcal{S}$. A multi-agent system reasoning process is expressed as:

$$\mathcal{Y} = \mathcal{F}(\mathcal{A}_1(\mathcal{Q}, \mathcal{S}), \mathcal{A}_2(\mathcal{Q}, \mathcal{S}), ..., \mathcal{A}_n(\mathcal{Q}, \mathcal{S}))$$

where $\mathcal{Y}$ stands for the final answer generated by the system. $\mathcal{A}_i(\mathcal{Q}, \mathcal{S})$ represents the answer of agent i, $\mathcal{F}$ stands for the communication protocol manually customized by the design of the system which aggregate the answer of each agents into the final answer. Typically, it could be majority vote, debate, etc (Kaesberg et al., 2025; Liu et al., 2024a). In our specific setup, we adopt a sequential processing communication mechanism inspired by Qian et al. (2024) to prevent context explosion (Liu et al., 2024b; Xu et al., 2024c). In this mechanism, for $i = 2, ..., n$, agent $\mathcal{A}_i$ receives the complete output generated by the immediately preceding agent $\mathcal{A}_{i-1}$. In contrast, from the preceding agents $\{\mathcal{A}_1, ..., \mathcal{A}_{i-2}\}$, $\mathcal{A}_i$ receives only the final answers. The detailed communication algorithm could be found in Appendix A Algorithm 1.

3.2 Dataset

For our experiments, we select four distinct domains from MMLU-pro (Wang et al., 2024d): Math, Health, Business, and Law. These four domains are selected for being representative and frequently studied in contemporary multi-agent reasoning research (Cui et al., 2023; Lei et al., 2024; Ghezloo et al., 2025). We further classify these four domains into three categories based on the primary reasoning type required: (1) **Mathematical Reasoning**: Domains requiring formal mathematical deduction to derive the answer. (2) **Factual Recall Reasoning**: Domains primarily requiring the recall of domain-specific factual knowledge, seldom needing extensive reasoning steps other than simple mathematical calculations. (3) **Contextual Reasoning**: Domains requiring not only the retrieval of relevant expert knowledge but also its application within the reasoning process of specific scenarios

or contexts. This choice of evaluation domains and fine-grained classification of their reasoning types allow us to investigate the effects of collaborative expertise specialization on multi-agent system from a more systematic manner.

3.3 Collaborative Expertise Specialization

In this paper, we primarily studied the effect of collaborative expertise specialization on better multi-agent system design from the perspective of expert-domain alignment, collaboration paradigms and system scale. To formalize the role and responsibility of the agents in the multi-agent system, we define each expert to be of the following format:

$$\mathcal{A}_i \leftarrow (EG, FR, R, ID)$$

where $\mathcal{A}_i$ stands for agent i, EG, FR and R represent Expert Group, Formal Role and Responsibility respectively. ID represents an agent's index within the group of all agents who share the same role.

3.4 General Experiment Setup

As detailed in Section 3.2, we select 4 representative domains from MMLU-pro to investigate the effects of collaborative expertise specialization. To be consistent with all experiments, we utilize DeepSeek-R1-Distill-Qwen-7B (DeepSeek-AI et al., 2025) as the foundational model for all agents. Each agent is initialized with its specific expert description and responsibilities via its system prompt, while the task instance is provided through the user prompt. The detailed prompts could be found in Appendix B. All experiments adopt accuracy as the evaluation metric.

4 Leveraging the "Right" Agent

Expertise specialization is a widely adopted technique in agent research, demonstrably enhancing the reasoning capabilities of LLMs within specific domains (Li et al., 2024b). While the benefits of specialization for individual agents are well-established, the effect of collaborative expertise specialization on the collective reasoning performance of multi-agent systems remains underexplored. This section presents our experimental investigation into this critical area, designed to unveil how different collaborative expertise specialization configurations influence the reasoning capabilities of multi-agent systems.

4.1 Setup

Considering the primary principle of multi-agent reasoning system is to incorporate more diverse agent viewpoints and integrate them in the final answer (Liang et al., 2024), in our experiments, we adopt diversity-driven collaboration paradigm where we distribute each agent with a specific domain expert configuration and instruct them to generate responses based on their expertise. At this stage, we fix the size of the multi-agent reasoning system to be 3 for controllable computational cost. We employ GPT-4o (OpenAI et al., 2024) for expert configuration generation. The detailed prompts utilized for this automated role generation process are provided in Appendix C.

4.2 "Right" Expertise Helps Reasoning

Our experiments demonstrate a clear performance advantage when the collaborative expertise specialization of the multi-agent system aligns with the domains of the downstream task. Misaligned expertise configurations often underperform compared to aligned ones. This primary finding is quantitatively supported by the results presented in Table 1. Specifically, in 75% of the aligned cases (diagonal entries), the system achieves the highest accuracy compared to configurations where the agent group simulates expertise from other domains for the same task.

To gain a more nuanced understanding of when expertise alignment is most beneficial, we analyze the system performance according to the primary reasoning type required by each domain, as categorized in Section 3.2. Our analysis reveals that the benefits of expertise alignment are most pronounced for tasks demanding contextual reasoning—Health and Law. Systems operating on these two domains exhibit an average relative performance improvement of 6.75% when expertise is correctly aligned, compared to the misaligned configurations which perform the second best for those tasks. Conversely, for domains requiring mathematical reasoning—Math and Business, the specialized experts yield only marginal gains or even degradation relative to misaligned configurations. We hypothesize this divergence stems from the inherent strengths of LLMs on math. These models often possess robust mathematical reasoning capabilities due to extensive pre-training, potentially reducing the added value of specialized agents. Contextual reasoning tasks, however, appear to benefit more

Dom.\Exp.	Math	Fina	Med	Law	Δ_h	Δ_{abs}
Math	**78.0**	76.3	76.3	76.4	2.1%	1.6 ↑
Business	**65.4**	64.3	62.4	62.4	-1.7%	1.1 ↓
Health	28.9	26.8	**30.4**	26.1	5.2%	1.5 ↑
Law	18.3	19.2	18.5	**20.8**	**8.3%**	1.6 ↑

Table 1: This table shows the impact of collaborative expertise specialization for different expert groups across various domains. "Dom." and "Exp." abbreviate Domain and Expert Group, respectively. $\Delta_{rel}/\Delta_{abs}$ indicate the relative/absolute performance improvement of the domain-aligned expert group compared to the best-performing alternative group respectively.

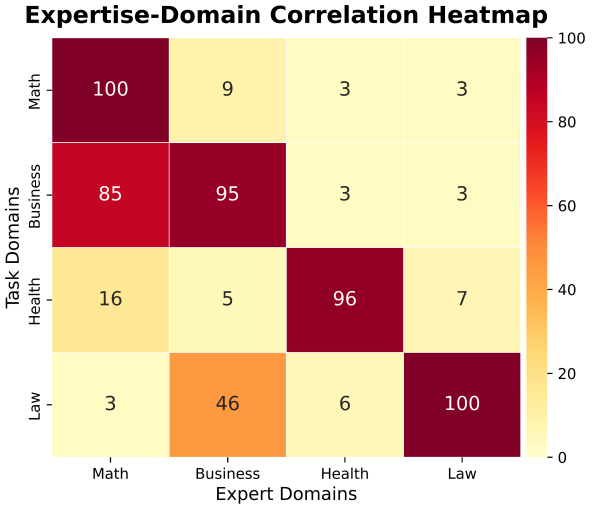

Figure 3: Heatmap illustrating the correlation between specialized group expertise and task domains. Deeper colors indicate stronger correlations.

from the structured integration of specialized perspectives provided by the multi-agent reasoning system since applying domain knowledge in these contexts often requires nuanced interpretation, synthesis of information, and reasoning beyond direct mathematical deduction.

4.3 Analysis on Expert-Domain Alignment

Furthermore, our experimental results reveal a positive correlation between how well the simulated group expertise aligns with the downstream task domain and the observed performance gain. This relationship is visualized in the expertise-domain correlation heatmap presented in Figure 3. Specifically, configurations where the simulated expertise is more relevant to the target task domain tend to yield greater performance improvements compared to less relevant configurations.

To quantify this expertise-task relevance, we first establish a relevance matrix. We randomly sample 100 instances from each of the four primary task domains. For each instance, we prompt Deepseek-V3 (DeepSeek-AI et al., 2025) to identify a list of 2-3 key expertise domains pertinent to solving the task. We then aggregate these identified candidate domains across all instances within each primary task domain. The relevance scores are calculated by counting the occurrences where a specific knowledge domain (e.g., Business) is deemed relevant for tasks in a primary domain (e.g., Math). These frequencies form a relevance matrix, visualized as a heatmap in Figure 3, where deeper color indicate higher relevance scores.

Comparing this relevance heatmap with the results in Table 1, we observe a consistent pattern supporting our initial finding—Higher expertise-domain relevance, indicated by deeper colors in the heatmap entries, generally corresponds to better reasoning performance. Many cells with high relevance scores in Figure 3 correspond to performance that are bolded or underlined in Table 1, signifying the best or second-best performance among group expertise specialization performance for that task domain. Conversely, low relevance scores typically correspond to misaligned configurations which barely demonstrate distinct advantages conferred by their specific (misaligned) expertise.

Our findings further support the established use of collective expertise specialization in multi-agent reasoning systems, while simultaneously highlighting the critical importance of aligning expertise design with the specific requirements of the target downstream domains, paving a fundamental guidance for future specialization technique application in multi-agent reasoning system design.

5 Structured Collaboration versus Diversified Discussion

A further critical consideration in multi-agent system design is the selection of an effective collaboration paradigm. Even when individual agents possess appropriate domain knowledge, the overarching mechanism governing their interaction can impact overall system performance. In this section, we present comparative experiments designed to analyze these distinct collaboration paradigms. Our objective is to investigate their potential advantages, thereby providing empirically grounded insights for effective collaboration paradigm choice in multi-agent system design.

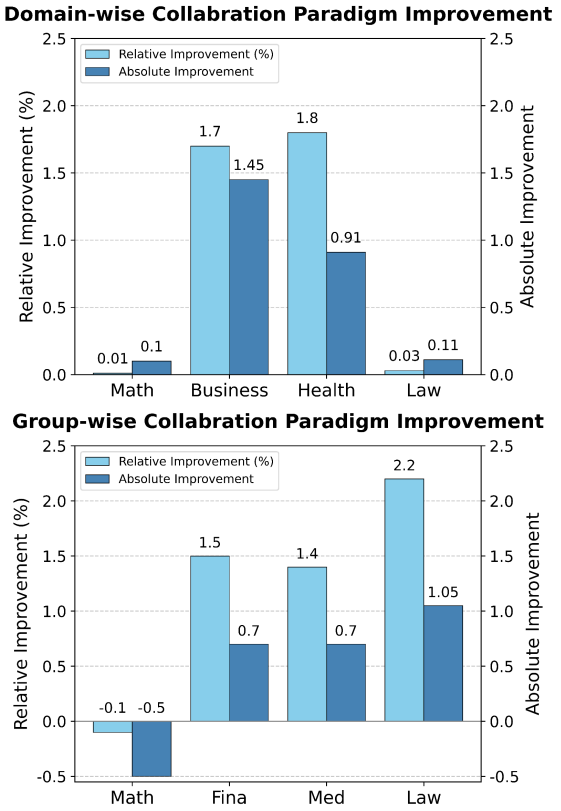

Figure 4: Comparative analysis of diversity-driven versus structured workflow collaboration paradigms. Positive values signify Diversity-Driven's advantage over Structured Workflow.

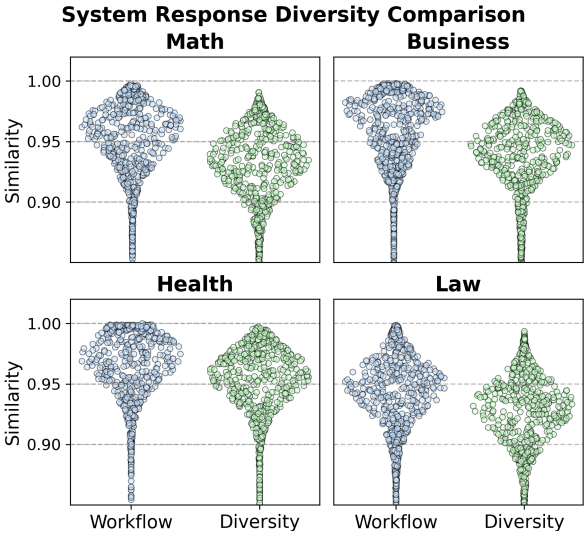

Figure 5: Illustration of response diversity across four distinct domains, where lower inter-agent response similarity corresponds to higher diversity.

5.1 Setup

Our analysis leverages the results presented in Figure 4, where we demonstrate both domain-wise and group-wise comparisons for a comprehensive overview. The detailed distinction between paradigms are illustrated as follows:

Diversity-Driven Collaboration: This paradigm emphasizes assigning agents highly specialized, fine-grained expertise within a broader domain (e.g., specific sub-fields of Laws). The objective is to foster collaboration through the integration of diverse, complementary knowledge perspectives during the reasoning process. Each agent contributes deep expertise from a narrow viewpoint.

Structured Workflow Collaboration: Conversely, this paradigm assigns roles based on distinct functional responsibilities within a predefined problem-solving process, in our case, solver, critic and coordinator. Collaboration centers on agents executing specific steps and refining intermediate outputs based on their functional role, rather than primarily contributing unique domain knowledge specializations. The differentiation between agents stems from their function within the workflow.

To ensure a plausible, accurate generation of expert role descriptions, we continue to employ GPT-4o with collaboration paradigm as extra input.

5.2 Diversity Matters in Collaboration

Our primary finding is that the diversity-driven paradigm generally yields superior performance compared to the structured workflow paradigm. This advantage holds true both when considering performance from both domain-wise and group-wise perspectives.

A domain-wise analysis, depicted in Figure 4, confirms this trend. Irrespective of the domain's primary reasoning type categorized in Section 3.2, the diversity-driven approach consistently results in performance gains over structured workflow. Notably, the most substantial improvements are observed in business and health domains, which demonstrate an average relative performance increase of 1.75% under diversity-driven paradigm. This indicates the potential of expertise with finer-granularity perform well across different domains.

Examining the results from group-wise perspective further supports this conclusion. With the exception of math expert group, all other specialized groups achieve higher average performance across all task domains when employing diversity-driven paradigm. When including the math group, the overall average relative performance improvement facilitated by the diversity-driven approach across all groups is 1.25%, indicating consistent benefits regardless of the task domain encountered.

Synthesizing these observations, the diversity-

driven collaboration paradigm demonstrates a consistent performance advantage over structured workflow collaboration paradigm across both different tested domains and distinct expertise configurations. This suggests that multi-agent systems could benefit significantly from collaboration structures that emphasize fine-grained expertise allocation which stimulates viewpoint diversity, providing a solid empirical basis for future research directions in designing multi-agent reasoning system's collaboration pattern.

5.3 Analysis on Response Diversity

To quantitatively characterize how the collaboration paradigm influences the diversity of agent contributions, we further design a response diversity analysis. We leverage semantic embeddings derived from Sentence-BERT (Reimers and Gurevych, 2019). For each task instance solved by the multi-agent system, we generate embeddings for the output of each agent. We then measure the internal diversity of the system's responses by calculating the pairwise cosine similarity between the embeddings of outputs from different agents. This provides a measure of how semantically distinct the contributions are at different stages.

The distributions of these pairwise similarity scores for both the diversity-driven and structured workflow paradigms are presented in Figure 5. The results clearly indicate that, the pairwise cosine similarity values are consistently lower for the diversity-driven collaboration paradigm compared to the structured workflow paradigm. This finding demonstrates that the diversity-driven approach, which emphasizes fine-grained expertise, fosters greater semantic diversity among agent responses throughout the collaborative reasoning, further confirming that enhancing the diversity of perspectives within a multi-agent system would be a key factor in improving its overall reasoning performance.

6 Scaling Up Reasoning Experts

Finally, the most complicated dimension in designing multi-agent systems to foster collective intelligence is the system scale. While the deployment of large-scale multi-agent systems for simulating social behaviors has received considerable attention, the implications of scaling under collaborative expertise specialization setup remain unexplored. This section details our investigation into the effects of varying system scale on both the reasoning performance of multi-agent systems and the associated computational trade-offs. We aim to elucidate how increasing the number of agents influences collective reasoning efficacy and to call for a better communication protocol design through our performance/token overhead trade-off analysis.

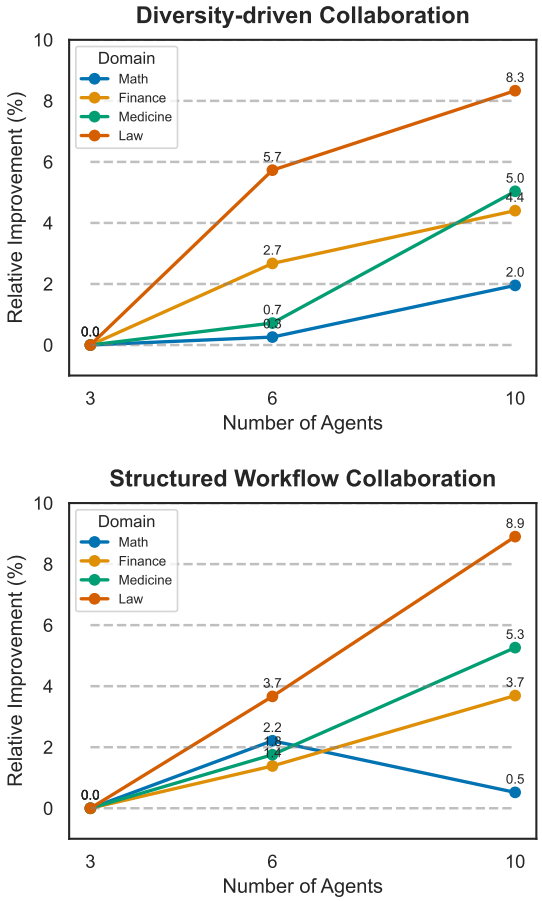

Figure 6: Domain-wise relative performance improvement by scaling up the multi-agent system (3, 6, and 10 agents), shown for different collaboration mechanisms.

6.1 Setup

We expand our experimental setup from 3 agents to systems comprising 6 and 10 agents. For these larger systems, we systematically replicate the experiments previously introduced, allowing for a direct comparison across different scales.

Generating coherent and appropriately specialized expert role configurations for these larger systems requires extending the initial configurations of the 3 agent system and we continue to leverage GPT-4o for this purpose. The detailed prompts employed for this role augmentation process are provided in Appendix C

6.2 More Experts, More Intelligent System

We evaluate the effect of system scale on reasoning performance by comparing the results from larger agent systems against the baseline 3 agent system. Specifically, we calculate the domain-wise relative performance difference for the system size of 6 and 10 with respect to system of size 3. These relative performance differences are illustrated in Figure 6.

Our findings reveal a consistent trend: increasing the number of agents generally enhances the multi-agent system's reasoning performance across the evaluated domains, regardless of whether diversity-driven or structured workflow paradigm is employed. However, the magnitude of this improvement varies significantly by domain. Corroborating our earlier observations regarding domain-specific analysis in Section 4, the performance gains within math domain are marginal, even when scaling up to 10 agents. Conversely, domains that necessitate substantial contextual reasoning and knowledge application demonstrate significantly larger performance improvements with increased system scale. This disparity suggests that the benefits derived from incorporating additional agents are most pronounced for tasks requiring the integration of diverse knowledge perspectives or complex, case-specific analysis inherent in non-mathematical reasoning. For domains characterized by intense mathematical reasoning, simply increasing the number of agents could barely yield diminishing returns. We believe our finding offers valuable insight for constructing large-scale multi-agent systems intended for diverse domains.

6.3 Token-Performance Trade-off

We further explore the token-performance trade-off inherent in scaling multi-agent reasoning systems by calculating the ratio of performance improvement over token overhead (PoT) with quantitative results presented in Figure 7. We use the sum of reasoning token and answer token for the calculation of token overhead. All the performance improvement and token consumption overhead are counted relatively against system of size 3.

Our analysis reveals distinct trends both across and within domains. Cross-domain comparisons demonstrate that tasks requiring substantial contextual reasoning, such as those in health and law, yield higher PoT ratios. This suggests that increasing agent collaboration is particularly beneficial in these areas, as greater token consumption during the reasoning process leads to higher performance improvements. Conversely, mathematical reasoning tasks exhibit only marginal performance gains with additional agents, which implies smaller ensembles can achieve comparable performance with lower computational overhead, making large-scale multi-agent systems unnecessary for these tasks.

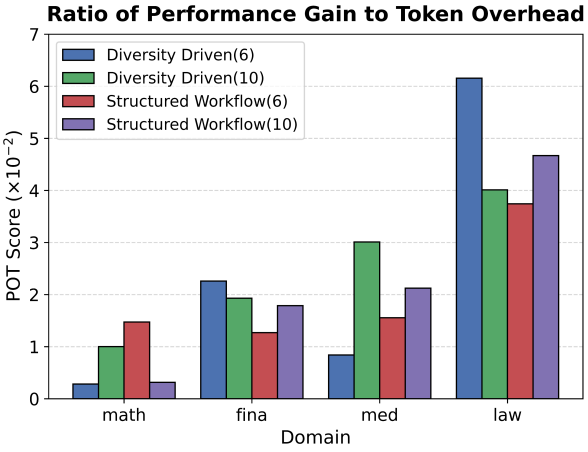

Figure 7: Performance improvement versus token overhead ratio across different domains. Both performance and token overhead are measured as relative increases compared to the system of size 3.

For intra-domain analysis, while structured workflows improved PoT in 75% of domains and diversity-driven approaches in 50% respectively, the critical finding is that neither collaboration paradigm guarantees an enhanced PoT across all domains tested. This widespread inconsistency in scaling behavior, regardless of the collaboration paradigm, highlights the pressing need for advancements in multi-agent communication protocols to achieve more stable and predictable performance enhancements as system complexity increases.

7 Conclusions

In conclusion, this paper systematically investigates the three factors of multi-agent system expertise specialization on collective reasoning intelligence: expertise-domain alignment, collaboration paradigm, and system scale. Our experiments verify the advantage brought by expertise specialization in multi-agent reasoning system, demonstrate the superiority of diversity-driven collaboration and indicate the existence of scaling law in multi-agent reasoning system with experts. These findings provide actionable insights for designing specialized multi-agent reasoning systems in future researches and underscore the need for developing more efficient coordination protocol as systems scale.

Limitations

Our adoption of MMLU-pro for evaluating specialized multi-agent reasoning system across diverse domains, while leveraging its strength in assessing varied domain-specific knowledge, inherently limits our assessment scope. Specifically, its focus on these reasoning paradigms means other crucial multi-agent capabilities, such as coding, might be overlooked. Apart from that, to enhance alignment with real-world scenarios, our evaluation concentrates on four key domains: Math, Business, Health, and Law, selected for their prominence in mainstream research. A direct limitation of this focused approach is that other potentially relevant domains would remain underexplored in the present study. Moreover, To simplify the research setup and promote more stable conclusions, we exclusively utilize one message propagation mechanism. This methodological choice, however, means that the potential influence of diverse communication strategies on system performance remains an unexplored aspect in our current study. Finally, We select DeepSeek-R1-Distilled-Qwen-7B as the base model for all experiments to ensure controllable computational overhead. This decision, while practical, limits our current investigation, deferring the study of multi-agent system architectures with larger-scale models to future research.

Ethics Statement

Our study involves publicly available datasets and use Large Language Models through APIs. Consequently, the ethical considerations of this paper could be listed as follow:

Datasets: We use publicly available datasets only for academic research purpose. We guarantee no personal data has been involved.

LLMs API: Our application of LLMs conform API provider's policy strictly, maintaining fair use and respecting intellectual property.

Transparency: We provide detailed descriptions of our method and the prompts used in our experiments, in line with standard practices in the research community. We will also make our code publicly available upon acceptance.

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Appendices

A Agent Communication Algorithm

In this section, we provide our detailed algorithm for inter-agent communication protocol and its corresponding notation table in below.

Algorithm 1 Communication Mechanism

procedure COLLABORATION($\mathcal{Q}, \mathcal{S}, \mathcal{M}_n$)
  for $\mathcal{A}_i$ in $\mathcal{M}_n$ **do**
    if i = n **then**
      $\mathcal{Y} \leftarrow \mathcal{A}_n(\mathcal{Q}, \mathcal{S}, \mathcal{A}_1, ..., \mathcal{A}_{n-1}^f)$
      return $\mathcal{Y}$
    else if i = 1 **then**
      $\mathcal{Y} \leftarrow \mathcal{A}_1(\mathcal{Q}, \mathcal{S})$
    else
      $\mathcal{Y} \leftarrow \mathcal{A}_i(\mathcal{Q}, \mathcal{S}, \mathcal{A}_1, ..., \mathcal{A}_{i-1}^f)$
    end if
  end for
end procedure

Symbol	Meaning
$\mathcal{A}_i$	The output without rationale of agent $\mathcal{A}_i$
$\mathcal{A}_i^f$	Full output with rationale of agent $\mathcal{A}_i$
$\mathcal{Q}$	Input question
$\mathcal{S}$	The candidate answers of the question
$\mathcal{Y}$	The final answer of the system

Table 2: Notation used in Algorithm 1

B Role System Prompt

In this section, we demonstrate the system prompt adopted for passing expertise role configuration and the user prompt for LLMs to receive the queries from MMLU-pro.

System Prompt

[ROLE ASSIGNMENT]

You are a {title} specializing in {domain}.
Your professional responsibility is to {duty}.
IMPORTANT: Think and respond EXACTLY as a real {title} in {domain} would.
Use terminology, methods, and perspectives specific to your professional field.

User Prompt

Previous discussion: {message_hist} PROBLEM TO SOLVE: problem RESPONSE INSTRUCTIONS: 1. Begin with: "As a {title} in {domain}, I..." 2. Analyze the problem using your professional expertise 3. Provide your expert recommendation 4. End with: "My answer is
boxed{{X}}" where X is the answer index
REQUIREMENTS: - Maintain your {title} perspective throughout - Use terminology from {domain} - Keep response under 150 words - Your answer MUST be in
boxed{{}} format
Remember: You are a {title}, not an AI assistant. Think and respond accordingly.

C Expert Generation Prompts

In this section, we provide the prompts used for expert configuration generation for multi-agent system of size 3 and prompts for expert configuration augmentation for system of size 6 and 10.

C.1 Primary Expert Generation Prompts

Prompt for Structured Workflow Expert Generation

Variables: {Domain}

Prompt: Generate me an expert group in Domain domain of size three, assigning them roles of solver, critic and coordinator together with their detailed responsibilities.

Prompt for Diversity-Driven Expert Generation

Variables: {Domain}

Prompt: Generate an expert group of size 3 in the Domain domain, each specializing in a distinct sub-domain of Domain. Provide a detailed configuration for each expert, including their role and responsibility, ensuring that their roles are complementary and collectively form a balanced, high-functioning team capable of addressing complex challenges in the domain. For example, an expert in a sub-domain of business could be “Global Compliance Architect”.

C.2 Expert Augmentation Process

Prompt for Structured Workflow Expert Augmentation

Variables: {Domain},{System Size},{Group Description of Size 3}

Prompt: Here is a expert group configuration in Domain domain of size 3: Group Description of Size 3.
Please augment the group size to System Size by assigning new experts with roles of solver, critic, strategist and coordinator. Output your configuration following the format of the given group configuration.

Prompt for Diversity-Driven Expert Augmentation

Variables: {Domain},{System Size},{Group Description of Size 3}

Prompt: Here is a expert group configuration in Domain domain of size 3: Group Description of Size 3.
Please augment the group size to System Size by assigning new experts with roles of expert in other sub-domains in Domain together with their responsibilities. Output your configuration following the format of the given group configuration.

D Social Group Role Examples

In this section, we present all the prompts for different expert agent groups of size 3 under different collaboration paradigms. The group under diversity-driven collaboration paradigm are exhibited in black while groups under structured workflow collaboration paradigm are shown in blue.

Math Group of 3

I. Differential Topologist

Responsibilities:
1. Analyze manifold embeddings using Whitney's conditions
2. Verify cobordism relations through Morse homology
3. Calculate characteristic classes via Čech-de Rham complexes

II. Proof Metrologist

Responsibilities:
1. Audit natural deduction derivations for intuitionistic consistency
2. Identify unstated ZFC dependencies
3. Verify category-theoretic diagram commutativity

III. Spectral Synthesizer

Responsibilities:
1. Decompose operator algebras using K-theory invariants
2. Construct Gelfand-Naimark-Segal representations
3. Analyze C*-algebra extension groups

Math Group of 3

I. Solver

Responsibilities:
execute core problem analysis using mathematical principles, formulate key equations, and establish foundational solution components with logical progression.

II. Critic

Responsibilities:
Analyze solution structure for conceptual consistency, identify invalid logical leaps, and verify fundamental mathematical truth of initial assumptions.

III. Coordinator

Responsibilities:
Integrate analytical components into unified framework, maintain mathematical coherence between steps, and prepare final solution presentation.

Finance Group of 3

I. Ethics & Compliance Officer

Responsibilities:
1. Merge UNGC/SBE mapping with FTC/ASA/CAP compliance
2. Conduct combined PESTEL/SWOT analyses
3. Integrate CSR violation detection with greenwashing audits
4. Handle stakeholder prioritization with power-interest matrices
5. Develop unified compliance solutions using BIA/GVV frameworks

II. Stakeholder Impact Strategist

Responsibilities:
1.Combine emotional valence analysis with reputational scoring
2.Merge Maslow's hierarchy applications with PROTECT framework
3.Manage supply chain/social impact predictions
4.Balance shareholder-stakeholder priorities
5.Coordinate multi-channel communication plans

III. Strategic Decision Leader

Responsibilities:
1.Integrate Monte Carlo simulations with game theory models
2.Oversee crisis protocol development/implementation
3.Manage alternative scenario planning
4.Conduct comprehensive risk-reward analysis
5.Finalize violation classifications/severity gradations

Finance Group of 3

I. Solver

Responsibilities:
Analyze regulatory compliance requirements, develop ethical frameworks, and optimize corporate governance strategies.

II. Critic

Responsibilities:
Evaluate stakeholder impact scenarios, identify compliance gaps, and verify ethical decision-making processes.

III. Coordinator

Responsibilities:
Integrate global compliance standards with local operations, balance stakeholder priorities, and ensure ethical crisis management.

Medical Group of 3

I. Disease Control Integrator

Responsibilities:
1.Combine SEIR modeling with transmission vector mapping
2.Merge clinical/public health intervention analysis
3.Integrate prevention frameworks with treatment protocols
4.Conduct combined cost-effectiveness/equity assessments
5.Develop unified outbreak response plans

II. Health Systems Engineer

Responsibilities:
1.Synthesize care delivery models with infrastructure analysis
2.Optimize vaccine protocols with screening algorithms
3.Manage digital health/supply chain integration
4.Balance individual/population health needs
5.Conduct pandemic preparedness simulations

III. Medical Priority Strategist

Responsibilities:
1.Reconcile SDG targets with local health realities
2.Apply GRADE criteria to population health approaches
3.Design risk-stratified intervention cascades
4.Finalize biological plausibility/scalability assessments
5.Produce multi-level prevention-treatment packages

Medical Group of 3

I. Solver

Responsibilities:
Analyze disease patterns and treatment effectiveness, develop care protocols, and optimize clinical workflows for patient outcomes.

II. Critic

Responsibilities:
Evaluate treatment safety and efficacy, identify gaps in care standards, and verify compliance with medical guidelines.

III. Coordinator

Responsibilities:
Integrate preventive care with treatment services, manage resource allocation, and ensure continuity of care across providers.

Law Group of 3

I. Contract Architect

Responsibilities:
1.Analyze UCC provisions vs common law principles
2.Identify material breach vs substantial performance
3.Map consideration adequacy through benefit-detriment analysis
4.Prepare parol evidence rule applicability matrix

II. Litigation Strategist

Responsibilities:
1.Develop FRCP-compliant pleading alternatives
2.Optimize discovery plan using proportionality standards
3.Calculate summary judgment probability scores
4.Prepare jury demand vs bench trial analysis

III. Regulatory Compliance Auditor

Responsibilities:
1.Conduct Chevron/Mead framework analysis
2.Map agency guidance through FOIA-obtained materials
3.Prepare preemption challenge vulnerability index
4.Maintain regulatory change tracking dashboard

Law Group of 3

I. Solver

Responsibilities:
Analyze contract validity and compliance, evaluate breach of duty scenarios, and develop legal documentation frameworks.

II. Critic

Responsibilities:
Audit regulatory adherence, identify compliance vulnerabilities, and verify proper application of legal precedents.

III. Coordinator

Responsibilities:
Integrate litigation strategies with dispute resolution mechanisms, balance evidentiary requirements, and ensure procedural compliance.

E Relevance Prompt

In this section, we provide the prompt used for generating related domain for queries in MMLU-pro. The generated related domains are then used for expertise-domain correlation heatmap generation.

Prompt for expertise-domain correlation analysis

You are an expert in identifying the domains of expertise required to solve a given problem. You will be provided with a question, and your task is to determine which domains from the following list are relevant: ['Math', 'Law', 'Business', 'Health'].
Please analyze the question and return the appropriate domains. There could be more than one domain that is necessary.
Please directly output a python list of the domains without other output.
Please limit your output to 2-3 domains.
For example: ['Med', 'Fina']
Please directly output the list that is loadable by python, no other output. 2-3 domains should be outputted, no more or less.

F All Experiments

In this section, we provide an overview of the experiment results across different expert groups and domains. The shadowed bars stand for the results of diversity-driven collaboration paradigm and the non-shadowed bars stand for the results of structured workflow collaboration paradigm.