



EIGEN-1: ADAPTIVE MULTI-AGENT REFINEMENT WITH MONITOR-BASED RAG FOR SCIENTIFIC REASONING

Xiangru Tang^{1,*}, Wanghan Xu^{2,*}, Yujie Wang^{1,*}, Zijie Guo^{3,*}, Daniel Shao¹, Jiapeng Chen¹, Cixuan Zhang¹, Ziyi Wang¹, Lixin Zhang¹, Guancheng Wan⁴, Wenlong Zhang⁶, Lei Bai⁶, Zhenfei Yin⁷, Philip Torr⁷, Hanrui Wang^{4,8}, Di Jin⁸

¹Yale University ²Shanghai Jiao Tong University ³Fudan University

⁴University of California, Los Angeles ⁶Shanghai AI Lab ⁷University of Oxford ⁸Eigen AI

ABSTRACT

Large language models (LLMs) have recently shown strong progress on scientific reasoning, yet two major bottlenecks remain. First, explicit retrieval fragments reasoning, imposing a hidden “tool tax” of extra tokens and steps. Second, multi-agent pipelines often dilute strong solutions by averaging across all candidates. We address these challenges with a unified framework that combines implicit retrieval and structured collaboration. At its foundation, a *Monitor-based retrieval module* operates at the token level, integrating external knowledge with minimal disruption to reasoning. On top of this substrate, *Hierarchical Solution Refinement (HSR)* iteratively designates each candidate as an anchor to be repaired by its peers, while *Quality-Aware Iterative Reasoning (QAIR)* adapts refinement to solution quality. On Humanits Last Exam (HLE) Bio/Chem Gold, our framework achieves 48.3% accuracy—the highest reported to date, surpassing the strongest agent baseline by 13.4 points and leading frontier LLMs by up to 18.1 points, while simultaneously reducing token usage by 53.5% and agent steps by 43.7%. Results on SuperGPQA and TRQA confirm robustness across domains. Error analysis shows that reasoning failures and knowledge gaps co-occur in over 85% of cases, while diversity analysis reveals a clear dichotomy: retrieval tasks benefit from solution variety, whereas reasoning tasks favor consensus. Together, these findings demonstrate how implicit augmentation and structured refinement overcome the inefficiencies of explicit tool use and uniform aggregation. The code is available at <https://github.com/tangxiangru/Eigen-1>.

1 INTRODUCTION

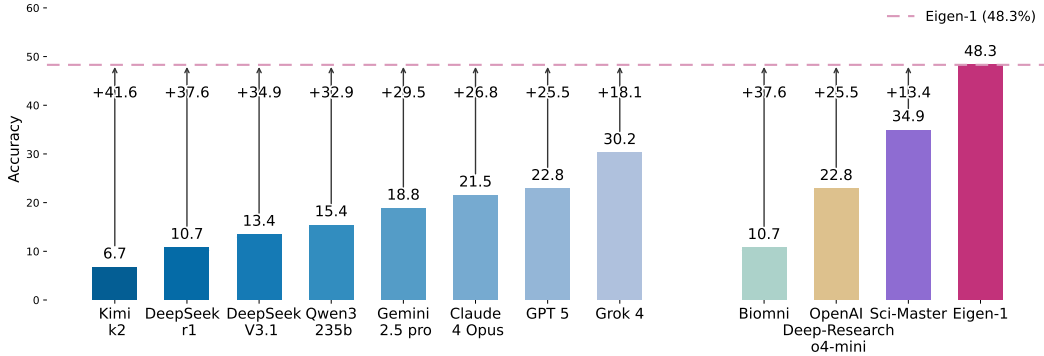


Figure 1: **HLE Bio/Chem Gold overall accuracy.** On the 149-problem HLE Bio/Chem Gold split (Pass@1, auto-judged by o3-mini), our system attains **48.3%** accuracy, exceeding the strongest agent baseline (SciMaster) by **+13.4** points and leading frontier LLMs by up to **+18.1** points.

*Equal contribution.

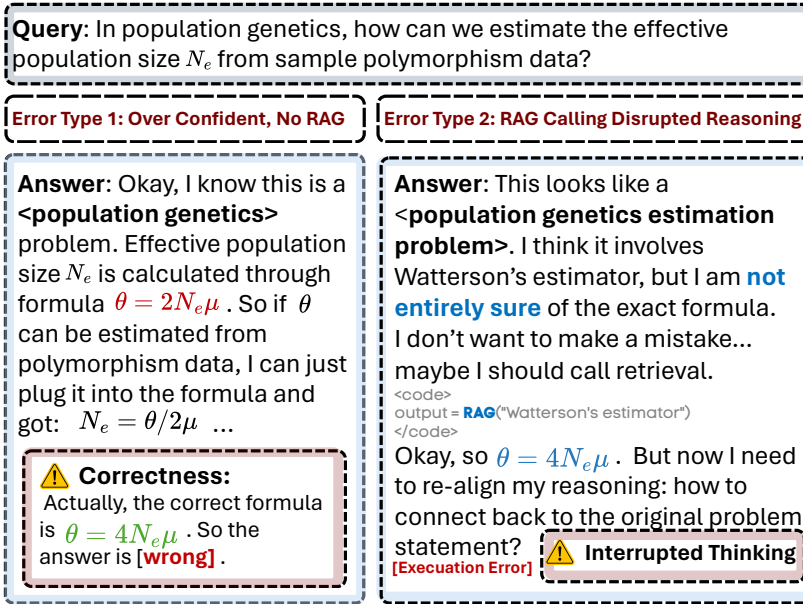


Figure 2: **Population genetics case with two failure modes.** *Left (Error Type 1):* the model confidently recalls an incorrect formula ($\theta = 2N_e\mu$) and derives $N_e = \theta/2\mu$, yielding the wrong answer. *Right (Error Type 2):* the model retrieves the correct relation ($\theta = 4N_e\mu$) via explicit RAG, but the reasoning flow is disrupted and the result is not reintegrated into the original problem, illustrating the *tool tax*. Our Monitor-based RAG avoids this context suspension by injecting the correct formula directly into the reasoning stream.

Recent advances in large language models have enabled impressive performance on a spectrum of reasoning benchmarks, from general-purpose evaluations such as MMLU [21] and mathematical problem solving [9; 43] to domain-specific tasks including ScienceQA [38], MedQA [29], and GPQA [42]. These results indicate that LLMs can already handle factual recall and mid-level reasoning across diverse domains. However, when moving to more demanding benchmarks such as Humanity’s Last Exam (HLE) [39; 47], which targets expert-level biology and chemistry problems, performance degrades substantially, and systematic failures persist when problems require deep domain knowledge and complex multistep reasoning [7]. Through comprehensive analysis of error patterns across 149 HLE Bio/Chem problems, we identify two fundamental architectural limitations: (1) *the fragmentation of logical flow through explicit tool invocation*, and (2) *the inefficiency of democratic multi-agent collaboration*.

Current retrieval-augmented generation systems [3; 19; 33] require explicit interruption to access external knowledge. Each retrieval breaks the reasoning flow: suspending the logical state, formulating queries, processing results, and reconstructing the context. This *tool tax* compounds quickly: solving population genetics problems requires Watterson estimators requires 8-10 such interruptions, doubling the number of agent steps compared to a baseline without information retrieval (see Table 3) while reducing coherence. The problem persists in all RAG paradigms: single-round approaches [1; 45] cannot adapt to emerging needs, iterative systems [27; 44] compound interruption costs, and reasoning-aware methods [51; 55] remain bound by explicit invocation, as shown in Figure 2.

Simultaneously, most current multi-agent systems [4; 52] employ rigid democratic workflows: generation, criticism, synthesis, selection, treating all solutions equally regardless of quality. This contradicts both cognitive science research on hierarchical expert reasoning [8; 32] and observations of scientific collaboration where ideas naturally organize into anchors and support [14]. Our analysis reveals that 92.8% of the failures involve reasoning errors, while 88.7% involve knowledge gaps, with substantial overlap, indicating that these challenges are fundamentally intertwined, as shown in Figure 7.

We present EIGEN-1, an efficient agent framework that unifies **Monitor-based RAG** eliminates *tool tax* through implicit augmentation, operating continuously at the token level to detect knowledge gaps via semantic uncertainty, generate contextual queries, and inject information seamlessly. **Hierarchical Solution Refinement (HSR)** rotates each candidate solution as an anchor and applies peer-informed repair from the remaining candidates, allowing structured cross-solution refinement rather than uniform averaging. **Quality-Aware Iterative Reasoning (QAIR)** replaces fixed workflows with adaptive cycles that respond dynamically to quality trajectories and problem characteristics. While our experiments focus on integration within a multi-agent reasoning framework, the design of Monitor-based RAG is

model-agnostic and can in principle be incorporated into other reasoning systems without architectural modification.

Our system achieves 48.3% accuracy in Humanity’s Last Exam Bio/Chem Gold, surpassing SciMaster [4] (34.9%) by 13.4 percentage points while reducing token consumption by 53.5% and agent steps by 43.7%. Solution pattern analysis further validates our framework: retrieval tasks benefit from diversity, whereas reasoning tasks favor consensus. These results demonstrate that eliminating the tool tax and embracing hierarchical collaboration enables both superior performance and computational efficiency, with potential implications that might extend beyond scientific reasoning to any domain requiring complex knowledge integration with logical inference.

2 RELATED WORK

2.1 EVOLUTION OF RETRIEVAL-AUGMENTED GENERATION

The integration of external knowledge into language model reasoning has evolved through three main paradigms. **Single-round RAG** systems [19; 25; 33] employ linear pipelines (rewrite→retrieve→generate) and are effective for factual queries. REALM [19] enabled end-to-end retrieval training, while RAG [33] extended this to knowledge-intensive tasks. More recent variants such as REPLUG [45] and In-Context RALM [41] improve robustness via black-box integration, but they lack adaptivity when knowledge needs emerge mid-reasoning. **Iterative RAG** introduces retrieval-generation loops for dynamic knowledge acquisition. ITER-RETGEN [44] alternates retrieval and generation, Self-RAG [1] uses self-reflection to decide retrieval, FLARE [27] predicts future content, and DRAGIN [48] updates datastores in real time. These improve grounding but typically incur $35\times$ more API calls. **Reasoning-aware RAG** embeds retrieval into reasoning itself. Chain-of-Note [57] produces reading notes, RAT [51] couples retrieval with thought generation, IRCOT [49] interleaves retrieval with chain-of-thought, and ReAct [54] unifies reasoning with action. While more integrated, they still depend on explicit tool calls, fragmenting reasoning and increasing latency.

Table 1 summarizes these paradigms against our Monitor-based approach. Unlike step-level methods that pause to query, Monitor-based RAG operates globally at the token level: it monitors uncertainty signals and implicitly injects evidence into context, reducing retrieval overhead while preserving reasoning continuity. Moreover, its retrieval granularity is finer, enabling more precise and frequent evidence integration without overwhelming the reasoning process.

Table 1: **RAG paradigms vs. key capabilities.** Single-round RAG is efficient but inadaptible; iterative RAG improves grounding but increases latency; reasoning-aware RAG offers tighter coupling yet still relies on explicit calls. **Monitor-based RAG** integrates evidence implicitly at the token level, improving continuity and efficiency.

System	Triggering	Fine-grained	Continuity	Efficiency	Adaptivity
Single-round RAG	✗	✗	✗	✓	✗
Iterative RAG	✓	✓	✗	✗	✓
Reasoning RAG	✓	✓	✓	✗	✓
Monitor-based RAG (Ours)	✓	✓	✓	✓	✓

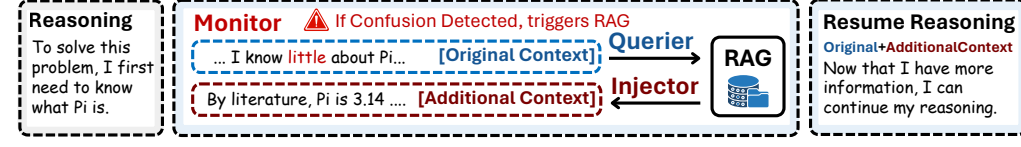
2.2 MULTI-AGENT REASONING SYSTEMS

Multi-agent frameworks have shown promise through collaborative problem solving, yet many rely on rigid orchestration assumptions.

Democratic collaboration systems treat all agents equally. SciMasters [4] employs solvercriticrewriter pipelines with a selector over candidate solutions, while LLM-Debate [13], Debate-Only-When-Necessary [15], and Multi-Agent Debate [35] use argumentative dialogue at different scales. MetaGPT [22] assigns role-based responsibilities, and CAMEL [34] explores autonomous cooperation. Table-Critic [56] extends these ideas to structured domains such as tabular reasoning. Such approaches, however, may devote substantial computation to low-quality candidates and do not explicitly capture hierarchical relationships among solutions.

Structured reasoning systems explore non-linear organizations. Tree-of-Thoughts [53] enables branching exploration with backtracking, Graph-of-Thoughts [2] allows arbitrary reasoning topologies, and Everything-of-Thoughts [11] combines multiple reasoning patterns. CoMM [5] introduces multi-path prompting, while HM-RAG [37] couples hierarchical agents with multimodal retrieval. Although these methods capture richer reasoning structures, they lack quality-aware adaptation and can rapidly expand search spaces.

(a) Monitor-based RAG



(b) Framework

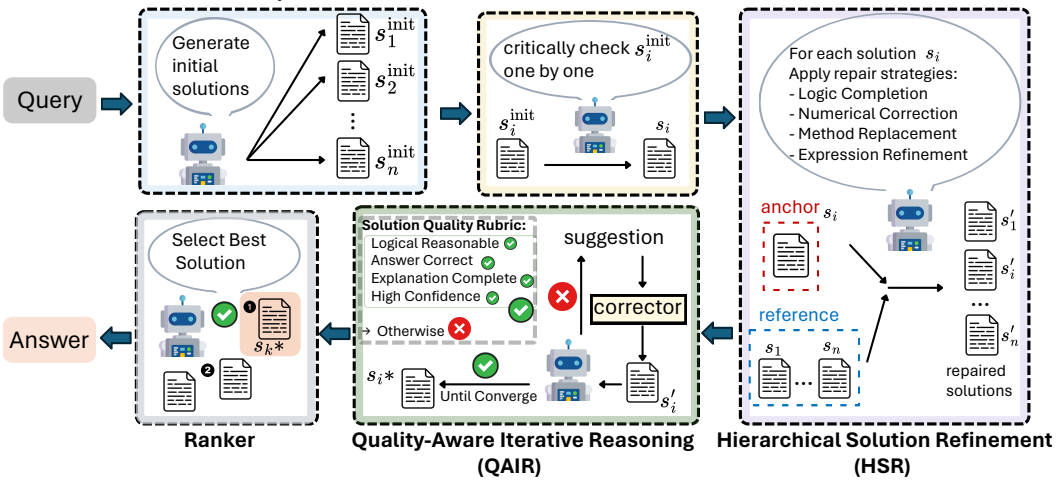


Figure 3: **Framework overview.** (a) *Monitor-based RAG* operates globally during reasoning: the Monitor detects insufficiency in the reasoning stream, the Querier generates targeted queries, and the Injector integrates retrieved evidence into context with minimal disruption. (b) Building on this substrate, the *Proposer* generates initial candidate solutions. Each candidate is revised individually by the *Corrector*, which applies local targeted fixes without access to other solutions. The improved candidates are then passed to *HSR*, which enables cross-solution refinement via anchor–reference relationships. Finally, *QAIR* evaluates overall quality and may invoke the *Corrector* again if needed, while the *Ranker* selects the strongest solution as the final answer.

Recent advances attempt more flexible or adaptive coordination. AgentVerse [6] supports dynamic team assembly, AutoGen [52] enables configurable conversation patterns, and Reflexion [46] incorporates self-improvement signals. Further, evolving orchestration [10], intent-propagation strategies [40], RL-enhanced planning with graph-based policies [26], and collaborative leader-follower training [16] highlight the need for adaptive depth and role specialization. Hierarchical orchestration frameworks such as AgentOrchestra [58] and HALO [23] exemplify this trend, emphasizing scalable coordination via layered or logic-oriented control.

In contrast, our HSR and QAIR modules introduce hierarchical refinement and quality-driven iteration. Rather than following critic–corrector or debate pipelines [35; 46; 52] that operate under democratic comment–rewrite loops and risk over-investing in weak candidates, HSR organizes solutions into anchor–reference structures for targeted repair, while QAIR applies quality-thresholded, suggestion-guided revisions with early stopping. Crucially, both mechanisms operate *on top of* monitor-based *implicit* RAG, enabling hierarchical, quality-aware convergence without suspending the reasoning process, echoing cognitive science findings on expert problem solving [8].

Declarative vs. Procedural Frameworks (DSPy vs. Ours) Declarative frameworks such as DSPy [31] compile tasks into prompt programs and retrieval policies, providing stability but with adaptation largely at the stage level. Our approach is procedural and run-time: a **Monitor**, **Querier**, and **Injector** operate during inference to adapt reasoning on the fly. This shift from compile-time templates to run-time control enables finer-grained adaptivity and seamless knowledge infusion.

3 METHOD

Overall workflow. EIGEN-1 integrates global retrieval, role-based reasoning, and higher-level refinement into a unified workflow, as shown in Figure 3 and Algorithm 1. Monitor-based RAG operates globally during reasoning: *Monitor* detects insufficiency in the reasoning stream, the *Querier* formulates targeted queries, and the *Injector* seamlessly integrates retrieved evidence back into context. Based on

this substrate, *Proposer* generates diverse candidate solutions, each of which is individually revised by *Corrector* through targeted local repairs. The refined candidates are then passed to *Hierarchical Solution Refinement (HSR)*, which introduces cross-solution repair through anchor-reference interactions. Next, *Quality-Aware Iterative Reasoning (QAIR)* evaluates overall quality and may invoke the corrector again for additional improvement. Finally, *Ranker* compares candidates and selects the strongest as the final solution. All agents can use web search tool (Serp API [30]) by default.

3.1 MONITOR-BASED RETRIEVAL-AUGMENTED GENERATION

Our Monitor-based RAG system augments reasoning implicitly, without fragmenting the workflow through explicit tool calls. Instead of forcing the LLM to pause, formulate a query, and inject evidence, the Monitor continuously inspects the reasoning trace, identifies potential knowledge insufficiencies, and invokes retrieval only when strictly necessary. The construction of the RAG database is shown in Appendix A.1.

3.1.1 MONITOR: DETECTING UNCERTAINTY AND TRIGGERING RETRIEVAL

The Monitor acts as a sentinel that periodically examines the reasoning trace and determines whether external knowledge is required:

$$\text{Monitor}(\text{context}) = \begin{cases} 1, & \text{if retrieval is required,} \\ 0, & \text{otherwise.} \end{cases}$$

Here, *context* refers to the partial reasoning sequence. Once insufficiency is detected, the retrieval is immediately triggered. To balance timeliness and efficiency, the Monitor runs in a streaming setup: It checks the reasoning at fixed intervals of 512 characters with an overlap of 128 characters. This overlapping design ensures that uncertainty markers that cross boundaries are not missed while keeping latency low. Details of RAG Monitor are in Appendix A.5.

3.1.2 QUERIER: IDENTIFYING UNCERTAINTY AND GENERATING TARGETED QUERIES

Triggered by the Monitor, the Querier converts the uncertain fragment into one or more retrieval queries: $[\text{query}_1, \dots, \text{query}_n] = \text{Querier}(\text{context})$. Here, the Querier maps the reasoning context into one or more concise, contextually appropriate queries. A key requirement of the Querier is to precisely extract the minimal set of keywords that capture the essential uncertainty in the reasoning trace. Depending on the task, this may result in a single keyword or a small collection of terms, each corresponding to a distinct retrieval perspective. The number and specificity of the generated queries directly determine the granularity of retrieval, which in turn controls the trade-off between recall and precision in RAG. By ensuring that queries are as fine-grained as possible, the Querier avoids unnecessary expansion of the search space while maximizing the relevance of retrieved evidence.

3.1.3 INJECTOR: EVIDENCE COMPRESSION AND CONTEXTUAL INTEGRATION

The Injector first filters and compresses raw RAG outputs into concise, utility-focused snippets to avoid redundancy and irrelevant noise. Then it rewrites and integrates the selected evidence in the Proposer’s reasoning context, ensuring coherence and preserving the natural flow of the reasoning narrative. This two-step design allows the knowledge retrieved to improve accuracy without introducing stylistic or structural disruptions: $\text{additional context} = \text{Injector}(\text{context}, \text{RAG results})$.

Figure 2 shows a population genetic problem that requires the Watterson estimator. Baseline LLMs exhibit two characteristic errors: (1) confidently recalling the wrong formula ($\theta = 2N_e\mu$) and deriving an incorrect effective population size, or (2) retrieving the correct formula ($\theta = 4N_e\mu$) via explicit RAG but failing to reintegrate it into the original reasoning chain, a classic case of *tool tax*. Our Monitor-based RAG resolves both issues: the Monitor detects semantic uncertainty, the Querier generates a targeted query, and the Injector seamlessly injects the correct formula into the reasoning stream, allowing the solution to proceed without disruption and converge to the correct answer, as shown in Figure 4.

3.2 HIERARCHICAL SOLUTION REFINEMENT (HSR)

HSR challenges the assumption that all solutions should contribute equally to the final output. Instead of democratic averaging, HSR establishes structured relationships among solutions that mirror expert collaboration patterns. Let $\mathcal{S} = \{s_1, \dots, s_n\}$ denote the candidate solutions. Each solution is iteratively designated as the anchor s_i , while the remaining set $\mathcal{R} = \mathcal{S} \setminus \{s_i\}$ provides references. This rotation ensures that every solution benefits from peer-informed repair, preventing premature convergence to a single trajectory.

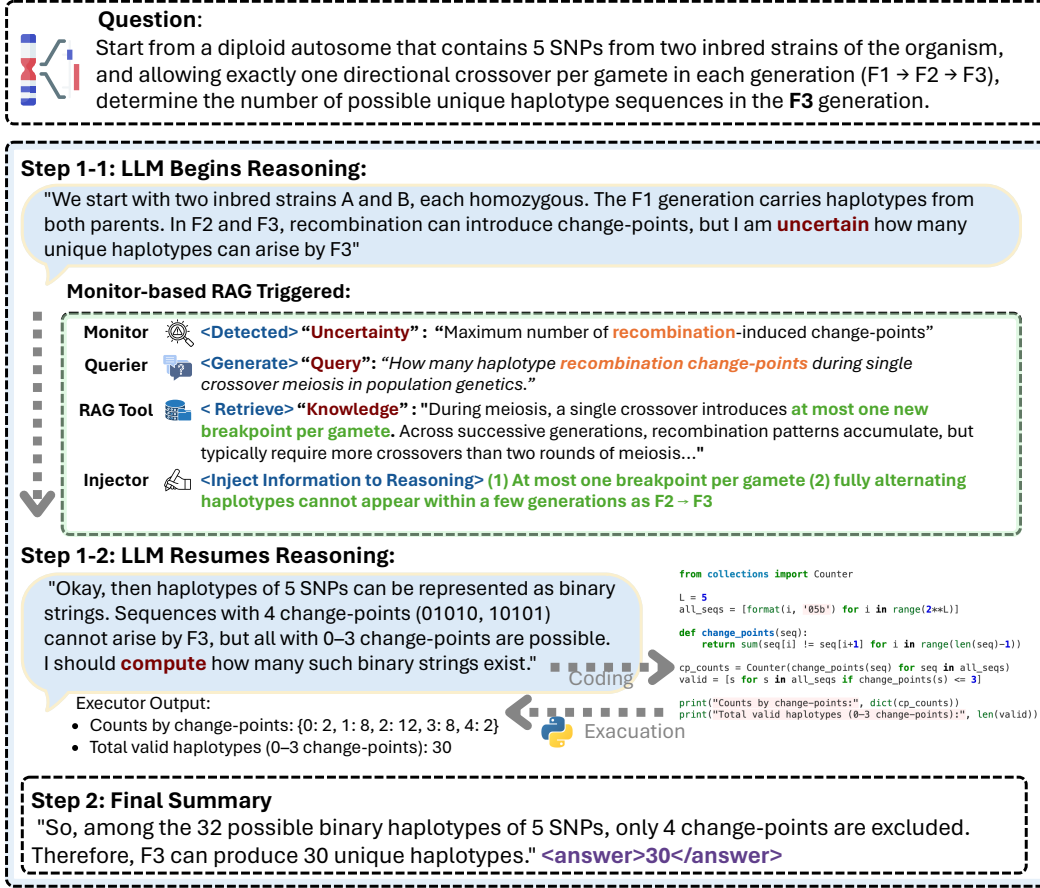


Figure 4: **Haplotype counting with single crossovers (F1→F3)**. The Proposer exhibits uncertainty about recombination constraints; *Monitor* detects insufficiency, *Querier* issues a targeted query, and *Injector* integrates two retrieved facts. This enables the reasoning to exclude invalid cases and converge on the correct count of 30 haplotypes.

Formally, the process can be described as $s'_i = \text{Refine}(s_i, \mathcal{R})$, where $\text{Refine}(\cdot)$ denotes the LLM-driven mechanism that applies multidimensional repairs to the anchor. Specifically, logical completion fills missing reasoning steps or implicit assumptions, numerical correction resolves arithmetic inaccuracies, method replacement substitutes stronger strategies for weaker ones, and expression refinement improves clarity without altering substance. These dimensions ensure that the weaknesses of the anchor are addressed systematically while preserving its original strengths.

Figure 5 shows a pathway reasoning problem where multiple proposers generate partial but inconsistent solutions. Baseline multi-agent synthesis averages across candidates, often propagating contradictions or omitting critical intermediates. Instead, HSR designates one solution as the anchor and integrates targeted corrections from reference solutions (e.g., filling in missing intermediates or fixing reaction links). This yields a coherent and biologically valid pathway, demonstrating how HSR consolidates fragmented contributions into a unified solution. QAIR then evaluates the refined set and can terminate the process once the quality stabilizes, avoiding unnecessary additional cycles.

3.3 QUALITY-AWARE ITERATIVE REASONING (QAIR)

QAIR introduces an evaluation-driven control mechanism to refine candidate solutions after the HSR stage. Let $\mathcal{S}' = \{s'_1, \dots, s'_n\}$ denote the initial set of refined candidate solutions. Each solution $s' \in \mathcal{S}'$ is evaluated by an LLM-based evaluator on three quality dimensions: logic, answer, and explanation, and a textual suggestion for improvement is generated. Each dimension is scored on a scale from 0 to 5, and the three quality scores are then combined into a composite score: $q(s') = 0.2 \cdot q_{\text{logic}}(s') + 0.6 \cdot q_{\text{answer}}(s') + 0.2 \cdot q_{\text{explanation}}(s')$, where the higher weight on the answer dimension emphasizes the correctness of the final answer while still allowing for logical consistency and explanatory clarity. Candidates meeting the threshold $\tau = 3$ are retained, while those failing are marked non-passing and passed to the corrector for targeted revision: $\tilde{s} = \text{Corrector}(s', \text{suggestion}(s'))$.

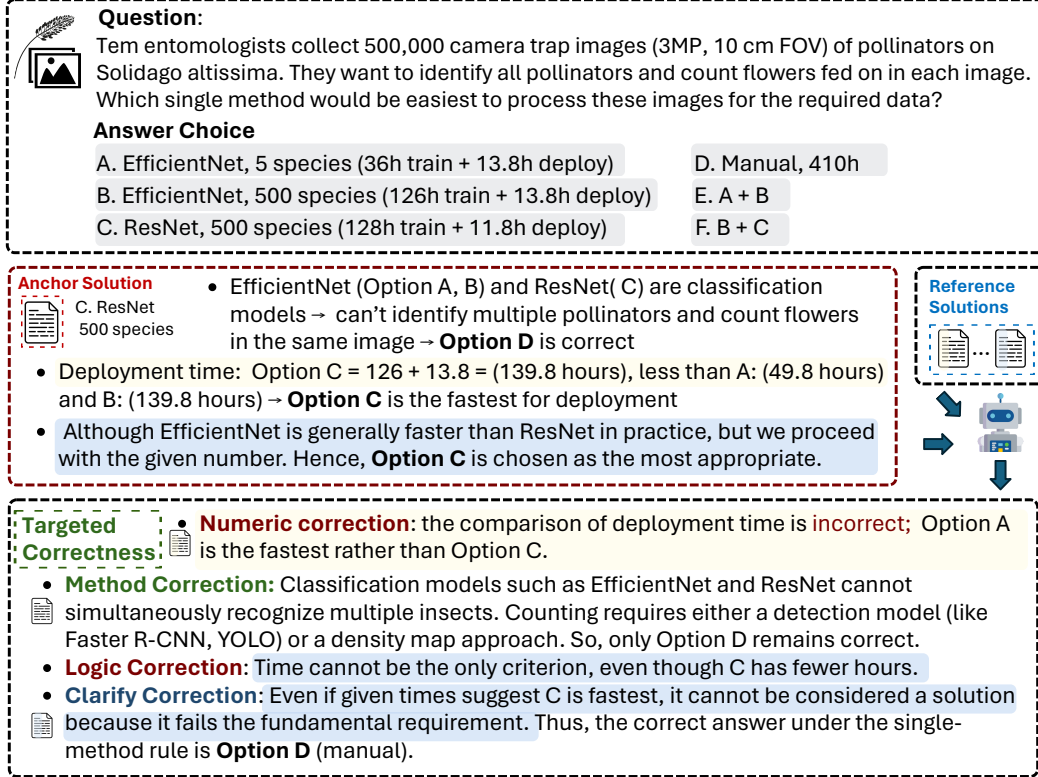


Figure 5: **Illustrative example: HSR.** The system rotates anchors among candidate solutions and integrates targeted corrections from references (e.g., fixing arithmetic mistakes, filling missing steps). Instead of averaging inconsistent candidates, HSR applies targeted improvements to yield a coherent final answer.

Let \mathcal{F}_t denote the set of solutions that fail the evaluation in round t , and \mathcal{E}_t denote the set of solutions evaluated at round t . Iterative refinement continues exclusively on the subset of failed solutions, forming the evaluation set for the next round $\mathcal{E}_{t+1} = \{\tilde{s} \mid s' \in \mathcal{F}_t\}$, until all solutions pass or maximum rounds T_{\max} is reached. By coupling structured quality assessment with suggestion-driven repair and avoiding re-evaluation of already validated candidates, QAIR efficiently converges toward a high-quality solution set while maintaining logical consistency, answer correctness, and explanatory clarity.

4 EXPERIMENTS

4.1 EXPERIMENTAL SETUP

We evaluate our approach on Humanity’s Last Exam (HLE) Bio/Chem Gold [47]¹, comprising 149 graduate-level problems in biology, medicine, and chemistry. HLE Bio/Chem Gold subset was manually curated and corrected by domain experts to ensure label fidelity. Additionally, we test on 92 hard-difficulty problems from SuperGPQA [12] Biology and 172 problems from TRQA Literature [59]. Our framework uses DeepSeek-V3.1 [36] as the base model with temperature 0.5 and 64K

Table 2: **Benchmark comparison under matched protocol.** HLE Bio/Chem (149 problems; o3-mini judge), SuperGPQA Biology (hard split), and TRQA Literature (multiple-choice).

Model	HLE Bio/Chem	SuperGPQA Hard	TRQA
<i>Base Models</i>			
Kimi K2	6.71	48.91	38.37
DeepSeek V3.1	13.42	66.30	43.60
Claude Opus 4.1	21.48	63.04	42.44
Gemini 2.5 Pro	18.79	65.22	45.93
GPT-5	22.82	61.96	50.58
Grok-4	30.20	66.30	46.51
<i>Agent Systems</i>			
SciMaster (GPT 4.1) [4]	9.45	19.78	47.67
Autogen (GPT 4.1) [52]	7.38	29.35	51.74
OpenAI Deep Research (o4-mini)	22.82	39.13	-
Biomni (GPT 4.1) [24]	10.74	43.48	41.09
SciMaster (DeepSeek V3.1)	34.92	66.30	51.74
EIGEN-1 (DeepSeek V3.1, Pass@1)	48.30	69.57	54.65
EIGEN-1 (DeepSeek V3.1, Pass@5)	61.74	78.26	79.07

¹<https://huggingface.co/datasets/futurehouse/hle-gold-bio-chem>

token limit. Following HLE protocol, we employ o3-mini for automated evaluation (See Appendix A.3). Beyond accuracy, we log total generated tokens and agent steps in the ablation experiments, as quantitative measures of the tool tax.

4.2 MAIN RESULTS

In the HLE Bio / Chem dataset, our system achieves **48.3%** accuracy (Pass@1), substantially outperforming the strongest baseline Grok-4 (30.2%) by nearly 18 absolute points and more than doubling the performance of general purpose models such as GPT-5 (22.8%) and Claude Opus 4.1 (21.5%). This margin is particularly notable, given that HLE problems require domain-specific reasoning rather than surface-level recall.

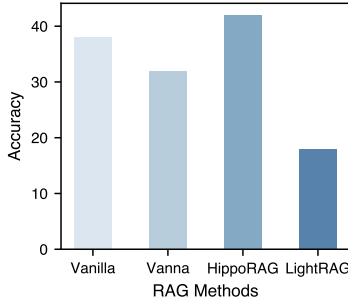
In SuperGPQA hard biology, our method reaches **69.6%**, exceeding all competing large models. The improvement is consistent across question categories, suggesting that our framework not only boosts correctness but also improves robustness on especially challenging scientific queries.

Finally, in TRQA benchmark, which emphasizes Information retrieval, integration and reasoning, our method obtains **54.7%** Pass@1, surpassing both Grok-4 (46.5%) and Gemini 2.5 Pro (45.9%). Furthermore, under the more permissive Pass@5, counting success if any of five attempts is correct, accuracy rises to **79.1%**, indicating robustness under a best-of-N setting.

Together, these results establish the advantage of our design in three heterogeneous benchmarks: biomedical, chemical and medical, demonstrating not only raw accuracy gains, but also improved adaptability across domains (Table 2). For more results of baseline models, please refer to Appendix A.7.

Within the Monitor-based RAG framework, we experimented with four retrieval backends: Vanilla [17], Vanna, HippoRAG [28], and LightRAG [18]. Among these, *HippoRAG* achieved the most consistent gains when coupled with our uncertainty detection. We attribute this to its finer-grained retrieval and graph-structured indexing, which better capture relevant context fragments without overwhelming the reasoning stream. Based on these results, we adopt HippoRAG as the default retrieval backend in our Monitor module (Figure 6).

Figure 6: Comparison of retrieval backends within Monitor-based RAG.



4.3 COMPONENT ANALYSIS

To understand the contribution of each architectural component, we performed systematic analysis on the full HLE Bio/Chem benchmark (149 problems), considering both incremental build-up and component ablation (Table 3).

The baseline configuration uses five parallel Proposers with access to a generic web search tool but without any paper retrieval (no RAG). The *Explicit* RAG setting adds a scientific paper database queried via embedding-based similarity. Unless otherwise noted, all settings use the same five-Proposer architecture with CriticCorrector refinement and Ranker selection.

The baseline system without external knowledge achieves 25.3% accuracy, underscoring the limitations of parametric knowledge alone for graduate-level science problems. Adding an explicit paper database improves accuracy to 41.4%, but at the cost of a sharp increase in workflow iterations (from 43.4 to 94.8). This reflects the high overhead of explicit retrieval: each tool call suspends reasoning, requires query formulation, and forces reintegration of results, fragmenting what should be a continuous reasoning flow. While the first one or two retrievals may be helpful, repeated interruptions often add little value and compound this “tool tax.”

Our Monitor-based RAG mitigates this overhead through implicit augmentation. By continuously monitoring generation and injecting knowledge only when necessary, it reduces token consumption by more than half (from 470.6K to 218.4K) and cuts workflow

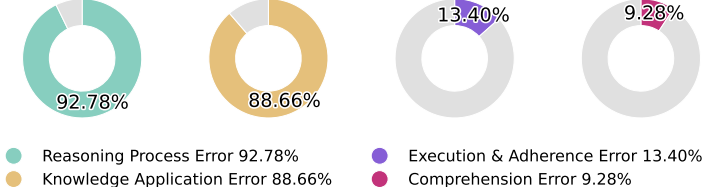


Figure 7: **Error type distribution.** Analysis of incorrect solution logs shows reasoning- and knowledge-related errors as dominant. Note that a single problem may involve multiple error types, so percentages do not sum to 100.

Table 3: **Component analysis from two perspectives on the full HLE Bio/Chem benchmark (149 problems)**. (a) Incremental build-up: modules are added one by one. (b) Component ablation: each module is removed from the full system. The baseline configuration uses five parallel Proposers with web search but without external paper retrieval (no RAG). *Steps* = agent-level workflow iterations (not token-level reasoning).

(a) Incremental build-up				(b) Component ablation			
Configuration	Accuracy (%)	Tokens (K)	Steps	Configuration	Accuracy (%)	Tokens (K)	Steps
Baseline (no ext. knowledge & no RAG)	25.3	483.6	43.4	Full system	48.3	218.9	53.4
+ Papers (Explicit RAG)	41.4	470.6	94.8	– (Monitor, Querier, Injector)	48.5	461.3	95.3
+ Monitor only	34.5	218.4	51.3	– Querier	45.9	224.1	53.1
+ Monitor + Querier	36.8	213.0	51.7	– Injector	44.7	202.5	52.1
+ Monitor + Querier + Injector	40.3	229.5	53.1	– HSR	44.8	234.1	53.5
+ Monitor + Querier + Injector + HSR	43.7	214.0	52.9	– QAIR	43.7	214.0	52.9
+ Monitor + Querier + Injector + HSR + QAIR	48.3	218.9	53.4				

iterations nearly in half (from 94.8 to 51.3), while maintaining competitive accuracy (34.5%). Adding the Querier improves query precision, leading to a modest gain to 36.8%. The limited margin compared to Monitor alone suggests that the primary bottleneck lies not in query formation but in evidence integration, which is addressed by the Injector. With the Injector, accuracy rises further to 40.3% with minimal additional overhead.

Hierarchical Solution Refinement (HSR) then contributes complementary gains, raising accuracy to 43.7%. Instead of naive aggregation, HSR leverages anchorreference interactions to apply targeted repairs, focusing revisions where they matter most (e.g., filling missing reasoning steps or correcting arithmetic). This adds some extra reasoning steps but yields proportionally higher accuracy.

Finally, Quality-Aware Iterative Reasoning (QAIR) builds on HSR by selectively invoking the Corrector when evaluation indicates further refinement is necessary. This yields the best overall result in the incremental sequence: 48.3% accuracy with 218.9K tokens and 53.4 iterations. Although QAIR introduces slight additional overhead, it ensures that every revision contributes meaningfully, preventing uncontrolled exploration or redundant cycles.

The ablation analysis further validates these findings: removing the Monitor results in a significant increase in the number of tokens and agent steps; and omitting HSR or QAIR lowers final performance to 44.8% and 43.7%, respectively. Together, these results show that Monitor-based RAG reduces the tool tax, HSR provides structured cross-solution repair, and QAIR ensures convergence through selective correction. Their combination achieves both state-of-the-art accuracy and controlled computation.

5 ANALYSIS

5.1 ERROR TYPE DISTRIBUTION

Analysis of failed problems reveals two dominant error modes: reasoning process errors (92.78%) and knowledge application errors (88.66%), as shown in Figure 7. These frequently co-occur, suggesting that successful scientific reasoning requires seamless integration of domain knowledge with logical inference. Execution errors (13.40%) and comprehension errors (9.28%) are comparatively rare, indicating that the primary challenge lies not in understanding problems or following instructions, but in maintaining coherent reasoning while accessing relevant knowledge. The strong overlap also suggests interdependence: missing knowledge often manifests as faulty reasoning steps, and disrupted reasoning in turn prevents effective incorporation of retrieved facts. For more examples of these different errors, see Appendix A.6.

5.2 DIVERSITY VS. CONSENSUS IN MULTI-AGENT SOLUTIONS

Our framework employs multiple parallel *Proposers* to generate candidate solutions and utilizes a *Ranker* to select the final answer. A natural assumption is that higher agreement among Proposers should correlate with higher accuracy. However, our analysis reveals a more nuanced picture: the relationship between solution diversity and correctness depends strongly on problem type.

To investigate this, we divide the benchmark into two categories: *information retrieval* tasks, which rely heavily on external knowledge, and *reasoning* tasks, which require longer chains of inference. For each problem, we measure the level of agreement among Proposers and evaluate how it correlates with accuracy. Both metrics are scored continuously by an LLM judge on a $[0, 1]$ scale: consistency reflects the pairwise agreement among candidate answers, while accuracy measures the graded alignment between a candidate and the ground-truth solution (see Appendix A.3). This continuous evaluation enables fine-grained correlation analysis beyond binary correctness. As shown in Fig 8, retrieval tasks benefit from diversity (low agreement), whereas reasoning tasks benefit from consensus (high agreement), with correlation slopes of 0.369 and 0.851, respectively.

This dichotomy suggests that different ranking strategies are optimal for different task types. In retrieval-heavy settings, the Ranker should preserve diversity and aggregate complementary perspectives, whereas in reasoning-heavy tasks, it should prioritize high-consensus answers as indicators of reliability. These observations highlight the complementary roles of HSR and QAIR, which operationalize the transition from diversity to consensus in a task-adaptive manner.

5.3 TOOL TAX QUANTIFICATION

The computational burden of explicit tool invocation extends beyond simple latency. As shown in Table 3, the *explicit RAG baseline* (with Proposers equipped with paper retrieval and web search) more than doubles agent-level workflow iterations compared to the no-IR setting ($43.4 \rightarrow 94.8$). This quantifies a hidden *tool tax* from context switching between reasoning and retrieval modes: each call requires the system to pause the evolving chain of thought, formulate a query, process external results, and then reconstruct the local context before continuing fragmenting what should be a continuous inference process.

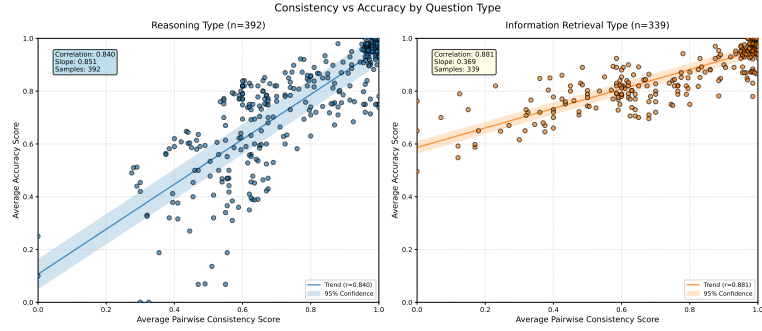


Figure 8: **Diversity vs. consensus.** Task-dependent effect of solution diversity: retrieval tasks benefit from variety, while reasoning tasks benefit from agreement. The horizontal axis reports the *average pairwise consistency score* among Proposers, computed by an LLM-based judge that evaluates semantic overlap between answers on a 0–1 scale. The vertical axis shows the *average accuracy score*, also judged by an LLM, which rates the degree of correctness of each answer relative to ground truth on a continuous 0–1 scale (rather than a binary 0/1). This continuous evaluation enables us to capture fine-grained trends between diversity and correctness across tasks. The fitted trend lines further highlight the contrast: retrieval tasks show a relatively flat slope (≈ 0.369), whereas reasoning tasks exhibit a much steeper positive slope (≈ 0.851), indicating a stronger dependence on consensus.

Fig. 9 visualizes this trade-off. Explicit RAG produces substantially longer traces without commensurate gains, whereas our *Monitor-based RAG* maintains concise, interpretable reasoning by injecting only the evidence that is needed, precisely when it is needed. Operating implicitly at generation time, it delivers comparable knowledge augmentation with markedly fewer tokens and iterations, avoiding repeated context suspensions.

More broadly, these findings argue for *implicit augmentation* and *adaptive tool policies* in agent design: systems should not treat all retrieval calls equally, but modulate retrieval frequency and depth based on emerging uncertainty, problem structure, and expected utility preserving continuity of reasoning while still accessing external knowledge when it truly helps.

6 CONCLUSION

Our experiments validate three key architectural innovations in EIGEN-1. First, implicit knowledge augmentation through Monitor-based RAG substantially reduces explicit retrieval overhead while preserving reasoning coherence. Second, HSR improves over uniform multi-agent aggregation by introducing structured anchor–reference relationships. Third, QAIR adaptively balances exploration and early stopping, achieving an effective trade-off between diversity and consensus. On HLE Bio/Chem, EIGEN-1 reaches 48.3% accuracy under compute-matched settings, with a 53.5% token reduction, showing that targeted architectural design can enhance both effectiveness and efficiency. By integrating external knowledge with minimal disruption to reasoning

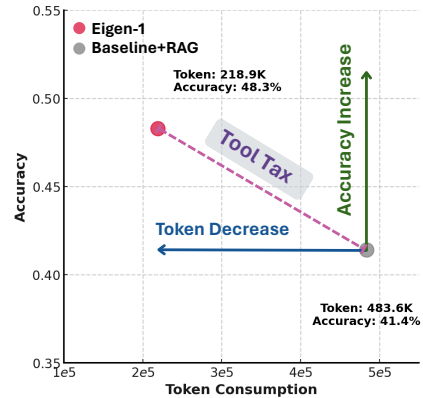


Figure 9: **Quantifying the tool tax.** Comparison of accuracy and coherence relative to compute cost, showing the overhead of explicit retrieval vs. implicit augmentation. Note that in this analysis, the baseline refers to the explicit RAG configuration (i.e., Proposers equipped with paper retrieval and web search), which represents the standard setup in most existing agent systems.

flow, our framework addresses key limitations of prior approaches in complex scientific problem solving. Future work will extend these principles to additional scientific domains, assess robustness and transferability, and explore integration into broader scientific workflows.

ETHICS STATEMENT

Our study aims to improve the scientific reasoning capabilities of large language models (LLMs) by introducing a unified framework that combines implicit retrieval and hierarchical collaboration. All datasets used in this work, including *Humanity’s Last Exam (HLE)*, *SuperGPQA*, and *TRQA*, are publicly available under open licenses. No private, sensitive, or human-identifiable data are involved. All annotations, where applicable, are derived from public benchmarks or generated using synthetic processes, ensuring that no ethical concerns regarding data privacy or misuse arise. The broader societal impact of this research lies in its potential to enhance scientific reasoning and complex problem-solving abilities in AI systems, which can be applied to fields such as education, scientific discovery, and decision support. Care has been taken to avoid overstating capabilities or drawing misleading conclusions, and we encourage further research to validate our findings across other high-stakes domains.

REPRODUCIBILITY STATEMENT

To ensure reproducibility, we provide detailed descriptions of our dataset preprocessing procedures, agent prompting strategies, and iterative refinement workflow in the appendix. These include full pipeline configurations and experimental setups required to reproduce the reported results with high fidelity.

REFERENCES

- [1] Akari Asai, Zeqiu Wu, Yizhong Wang, Avirup Sil, and Hannaneh Hajishirzi. Self-rag: Learning to retrieve, generate, and critique through self-reflection. 2024.
- [2] Maciej Besta, Nils Blach, Ales Kubicek, Robert Gerstenberger, Michal Podstawski, Lukas Gianinazzi, Joanna Gajda, Tomasz Lehmann, Hubert Niewiadomski, Piotr Nyczyk, et al. Graph of thoughts: Solving elaborate problems with large language models. In *Proceedings of the AAAI conference on artificial intelligence*, volume 38, pp. 17682–17690, 2024.
- [3] Sebastian Borgeaud, Arthur Mensch, Jordan Hoffmann, Trevor Cai, Eliza Rutherford, Katie Millican, George Bm Van Den Driessche, Jean-Baptiste Lespiau, Bogdan Damoc, Aidan Clark, et al. Improving language models by retrieving from trillions of tokens. In *International conference on machine learning*, pp. 2206–2240. PMLR, 2022.
- [4] Jingyi Chai, Shuo Tang, Rui Ye, Yuwen Du, Xinyu Zhu, Mengcheng Zhou, Yanfeng Wang, Yuzhi Zhang, Linfeng Zhang, Siheng Chen, et al. Scimaster: Towards general-purpose scientific ai agents, part i. x-master as foundation: Can we lead on humanity’s last exam? *arXiv preprint arXiv:2507.05241*, 2025.
- [5] Pei Chen, Boran Han, and Shuai Zhang. Comm: Collaborative multi-agent, multi-reasoning-path prompting for complex problem solving. *arXiv preprint arXiv:2404.17729*, 2024.
- [6] Weize Chen, Yusheng Su, Jingwei Zuo, Cheng Yang, Chenfei Yuan, Chen Qian, Chi-Min Chan, Yujia Qin, Yaxi Lu, Ruobing Xie, et al. Agentverse: Facilitating multi-agent collaboration and exploring emergent behaviors in agents. *arXiv preprint arXiv:2308.10848*, 2(4):6, 2023.
- [7] Ziru Chen, Shijie Chen, Yuting Ning, Qianheng Zhang, Boshi Wang, Botao Yu, Yifei Li, Zeyi Liao, Chen Wei, Zitong Lu, et al. Scienceagentbench: Toward rigorous assessment of language agents for data-driven scientific discovery. *arXiv preprint arXiv:2410.05080*, 2024.
- [8] Michelene TH Chi, Paul J Feltovich, and Robert Glaser. Categorization and representation of physics problems by experts and novices. *Cognitive science*, 5(2):121–152, 1981.
- [9] Karl Cobbe, Vineet Kosaraju, Mohammad Bavarian, Mark Chen, Heewoo Jun, Lukasz Kaiser, Matthias Plappert, Jerry Tworek, Jacob Hilton, Reiichiro Nakano, et al. Training verifiers to solve math word problems. *arXiv preprint arXiv:2110.14168*, 2021.
- [10] Yufan Dang et al. Multi-agent collaboration via evolving orchestration. *arXiv preprint arXiv:2505.19591*, 2025.
- [11] Ruomeng Ding, Chaoyun Zhang, Lu Wang, Yong Xu, Minghua Ma, Wei Zhang, Si Qin, Saravan Rajmohan, Qingwei Lin, and Dongmei Zhang. Everything of thoughts: Defying the law of penrose triangle for thought generation. *arXiv preprint arXiv:2311.04254*, 2023.

-
- [12] Xinrun Du, Yifan Yao, Kaijing Ma, Bingli Wang, Tianyu Zheng, King Zhu, Minghao Liu, Yiming Liang, Xiaolong Jin, Zhenlin Wei, et al. Supergpqa: Scaling llm evaluation across 285 graduate disciplines. *arXiv preprint arXiv:2502.14739*, 2025.
 - [13] Yilun Du, Shuang Li, Antonio Torralba, Joshua B Tenenbaum, and Igor Mordatch. Improving factuality and reasoning in language models through multiagent debate. In *Forty-first International Conference on Machine Learning*, 2023.
 - [14] Kevin Dunbar. How scientists think: On-line creativity and conceptual change in science. 1997.
 - [15] Sugyeong Eo, Hyeonseok Moon, Evelyn Hayoon Zi, Chanjun Park, and Heuseok Lim. Debate only when necessary: Adaptive multiagent collaboration for efficient llm reasoning. *arXiv preprint arXiv:2504.05047*, 2025.
 - [16] Andrew Estornell et al. How to train a leader: Hierarchical reasoning in multi-agent llms. *arXiv preprint arXiv:2507.08960*, 2025.
 - [17] Yunfan Gao, Yun Xiong, Xinyu Gao, Kangxiang Jia, Jinliu Pan, Yuxi Bi, Yixin Dai, Jiawei Sun, Haofen Wang, and Haofen Wang. Retrieval-augmented generation for large language models: A survey. *arXiv preprint arXiv:2312.10997*, 2(1), 2023.
 - [18] Zirui Guo, Lianghao Xia, Yanhua Yu, Tu Ao, and Chao Huang. Lightrag: Simple and fast retrieval-augmented generation.(2024). *arXiv preprint arXiv:2410.05779*, 2024.
 - [19] Kelvin Guu, Kenton Lee, Zora Tung, Panupong Pasupat, and Mingwei Chang. Retrieval augmented language model pre-training. In *International conference on machine learning*, pp. 3929–3938. PMLR, 2020.
 - [20] Conghui He, Wei Li, Zhenjiang Jin, Chao Xu, Bin Wang, and Dahua Lin. Opendatalab: Empowering general artificial intelligence with open datasets. *arXiv preprint arXiv:2407.13773*, 2024.
 - [21] Dan Hendrycks, Collin Burns, Steven Basart, Andy Zou, Mantas Mazeika, Dawn Song, and Jacob Steinhardt. Measuring massive multitask language understanding. *arXiv preprint arXiv:2009.03300*, 2020.
 - [22] Sirui Hong, Mingchen Zhuge, Jonathan Chen, Xiawu Zheng, Yuheng Cheng, Ceyao Zhang, Jinlin Wang, Zili Wang, Steven Ka Shing Yau, Zijuan Lin, et al. Metagpt: Meta programming for a multi-agent collaborative framework. *International Conference on Learning Representations, ICLR*, 2024.
 - [23] Zhipeng Hou, Junyi Tang, and Yipeng Wang. Halo: Hierarchical autonomous logic-oriented orchestration for multi-agent llm systems. *arXiv preprint arXiv:2505.13516*, 2025.
 - [24] Kexin Huang, Serena Zhang, Hanchen Wang, Yuanhao Qu, Yingzhou Lu, Yusuf Roohani, Ryan Li, Lin Qiu, Gavin Li, Junze Zhang, et al. Biomni: A general-purpose biomedical ai agent. *biorxiv*, 2025.
 - [25] Gautier Izacard and Edouard Grave. Leveraging passage retrieval with generative models for open domain question answering. *arXiv preprint arXiv:2007.01282*, 2020.
 - [26] Ziqi Jia, Junjie Li, Xiaoyang Qu, and Jianzong Wang. Enhancing multi-agent systems via reinforcement learning with llm-based planner and graph-based policy. *arXiv preprint arXiv:2503.10049*, 2025.
 - [27] Zhengbao Jiang, Frank F Xu, Luyu Gao, Zhiqing Sun, Qian Liu, Jane Dwivedi-Yu, Yiming Yang, Jamie Callan, and Graham Neubig. Active retrieval augmented generation. In *Proceedings of the 2023 Conference on Empirical Methods in Natural Language Processing*, pp. 7969–7992, 2023.
 - [28] Bernal Jimenez Gutierrez, Yiheng Shu, Yu Gu, Michihiro Yasunaga, and Yu Su. Hipporag: Neurobiologically inspired long-term memory for large language models. *Advances in Neural Information Processing Systems*, 37:59532–59569, 2024.
 - [29] Qiao Jin, Bhuwan Dhingra, Zhengping Liu, William W Cohen, and Xinghua Lu. What disease does this patient have? a large-scale open domain question answering dataset from medical exams. In *Proceedings of the Conference on Empirical Methods in Natural Language Processing (EMNLP)*, pp. 2397–2407, 2021.

-
- [30] Nils Kautto Ernberg. Analyzing google serp: Swedish search queries, 2019.
- [31] Omar Khattab, Arnav Singhvi, Paridhi Maheshwari, Zhiyuan Zhang, Keshav Santhanam, Sri Vardhamanan, Saiful Haq, Ashutosh Sharma, Thomas T Joshi, Hanna Moazam, et al. Dspy: Compiling declarative language model calls into self-improving pipelines. *arXiv preprint arXiv:2310.03714*, 2023.
- [32] Jill Larkin, John McDermott, Dorothea P Simon, and Herbert A Simon. Expert and novice performance in solving physics problems. *Science*, 208(4450):1335–1342, 1980.
- [33] Patrick Lewis, Ethan Perez, Aleksandra Piktus, Fabio Petroni, Vladimir Karpukhin, Naman Goyal, Heinrich Küttler, Mike Lewis, Wen-tau Yih, Tim Rocktäschel, et al. Retrieval-augmented generation for knowledge-intensive nlp tasks. *Advances in neural information processing systems*, 33:9459–9474, 2020.
- [34] Guohao Li, Hasan Hammoud, Hani Itani, Dmitrii Khizbullin, and Bernard Ghanem. Camel: Communicative agents for” mind” exploration of large language model society. *Advances in Neural Information Processing Systems*, 36:51991–52008, 2023.
- [35] Tian Liang, Zhiwei He, Wenxiang Jiao, Xing Wang, Yan Wang, Rui Wang, Yujiu Yang, Shuming Shi, and Zhaopeng Tu. Encouraging divergent thinking in large language models through multi-agent debate. *arXiv preprint arXiv:2305.19118*, 2023.
- [36] Aixiu Liu, Bei Feng, Bing Xue, Bingxuan Wang, Bochao Wu, Chengda Lu, Chenggang Zhao, Chengqi Deng, Chenyu Zhang, Chong Ruan, et al. Deepseek-v3 technical report. *arXiv preprint arXiv:2412.19437*, 2024.
- [37] Pei Liu et al. Hm-rag: Hierarchical multi-agent multimodal retrieval augmented generation. *arXiv preprint arXiv:2504.12330*, 2025.
- [38] Pan Lu, Swaroop Mishra, Tanglin Xia, Liang Qiu, Kai-Wei Chang, Song-Chun Zhu, Oyvind Tafjord, Peter Clark, and Ashwin Kalyan. Learn to explain: Multimodal reasoning via thought chains for science question answering. *Advances in Neural Information Processing Systems*, 35: 2507–2521, 2022.
- [39] Long Phan, Alice Gatti, Ziwen Han, Nathaniel Li, Josephina Hu, Hugh Zhang, Chen Bo Calvin Zhang, Mohamed Shaaban, John Ling, Sean Shi, et al. Humanity’s last exam. *arXiv preprint arXiv:2501.14249*, 2025.
- [40] Xihe Qiu, Haoyu Wang, Xiaoyu Tan, et al. Towards collaborative intelligence: Propagating intentions and reasoning for multi-agent coordination with large language models. *arXiv preprint arXiv:2407.12532*, 2024.
- [41] Ori Ram, Yoav Levine, Itay Dalmedigos, Dor Muhlgay, Amnon Shashua, Kevin Leyton-Brown, and Yoav Shoham. In-context retrieval-augmented language models. *Transactions of the Association for Computational Linguistics*, 11:1316–1331, 2023.
- [42] David Rein, Betty Li Hou, Asa Cooper Stickland, Jackson Petty, Richard Yuanzhe Pang, Julien Dirani, Julian Michael, and Samuel R Bowman. Gpqa: A graduate-level google-proof q&a benchmark. In *First Conference on Language Modeling*, 2024.
- [43] David Saxton, Edward Grefenstette, Felix Hill, and Pushmeet Kohli. Analysing mathematical reasoning abilities of neural models. In *International Conference on Learning Representations (ICLR)*, 2019.
- [44] Zhihong Shao, Yeyun Gong, Yelong Shen, Minlie Huang, Nan Duan, and Weizhu Chen. Enhancing retrieval-augmented large language models with iterative retrieval-generation synergy. *arXiv preprint arXiv:2305.15294*, 2023.
- [45] Weijia Shi, Sewon Min, Michihiro Yasunaga, Minjoon Seo, Rich James, Mike Lewis, Luke Zettlemoyer, and Wen-tau Yih. Replug: Retrieval-augmented black-box language models. *arXiv preprint arXiv:2301.12652*, 2023.
- [46] Noah Shinn, Federico Cassano, Ashwin Gopinath, Karthik Narasimhan, and Shunyu Yao. Reflexion: Language agents with verbal reinforcement learning. *Advances in Neural Information Processing Systems*, 36:8634–8652, 2023.

-
- [47] Michael Skarlinski, Jon Laurent, Albert Bou, and Andrew White. About 30% of humanity's last exam chemistry/biology answers are likely wrong. <https://www.futurehouse.org/research-announcements/hle-exam>, July 2025. Accessed: 2025-09-23.
- [48] Weihang Su, Yichen Tang, Qingyao Ai, Zhijing Wu, and Yiqun Liu. Dragin: dynamic retrieval augmented generation based on the information needs of large language models. *arXiv preprint arXiv:2403.10081*, 2024.
- [49] Harsh Trivedi, Niranjan Balasubramanian, Tushar Khot, and Ashish Sabharwal. Interleaving retrieval with chain-of-thought reasoning for knowledge-intensive multi-step questions. *arXiv preprint arXiv:2212.10509*, 2022.
- [50] Bin Wang, Chao Xu, Xiaomeng Zhao, Linke Ouyang, Fan Wu, Zhiyuan Zhao, Rui Xu, Kaiwen Liu, Yuan Qu, Fukai Shang, et al. Mineru: An open-source solution for precise document content extraction. *arXiv preprint arXiv:2409.18839*, 2024.
- [51] Zihao Wang, Anji Liu, Haowei Lin, Jiaqi Li, Xiaojian Ma, and Yitao Liang. Rat: Retrieval augmented thoughts elicit context-aware reasoning in long-horizon generation. *arXiv preprint arXiv:2403.05313*, 2024.
- [52] Qingyun Wu, Gagan Bansal, Jieyu Zhang, Yiran Wu, Beibin Li, Erkang Zhu, Li Jiang, Xiaoyun Zhang, Shaokun Zhang, Jiale Liu, et al. Autogen: Enabling next-gen llm applications via multi-agent conversations. In *First Conference on Language Modeling*, 2024.
- [53] Shunyu Yao, Dian Yu, Jeffrey Zhao, Izhak Shafran, Tom Griffiths, Yuan Cao, and Karthik Narasimhan. Tree of thoughts: Deliberate problem solving with large language models. *Advances in neural information processing systems*, 36:11809–11822, 2023.
- [54] Shunyu Yao, Jeffrey Zhao, Dian Yu, Nan Du, Izhak Shafran, Karthik Narasimhan, and Yuan Cao. React: Synergizing reasoning and acting in language models. In *International Conference on Learning Representations (ICLR)*, 2023.
- [55] Ori Yoran, Tomer Wolfson, Ori Ram, and Jonathan Berant. Making retrieval-augmented language models robust to irrelevant context. *arXiv preprint arXiv:2310.01558*, 2023.
- [56] Peiying Yu, Guoxin Chen, and Jingjing Wang. Table-critic: A multi-agent framework for collaborative criticism and refinement in table reasoning. *arXiv preprint arXiv:2502.11799*, 2025.
- [57] Wenhao Yu, Hongming Zhang, Xiaoman Pan, Kaixin Ma, Hongwei Wang, and Dong Yu. Chain-of-note: Enhancing robustness in retrieval-augmented language models. *arXiv preprint arXiv:2311.09210*, 2023.
- [58] Wentao Zhang et al. Agentorchestra: A hierarchical multi-agent framework for general-purpose task solving. *arXiv preprint arXiv:2506.12508*, 2025.
- [59] Zhongyue Zhang, Zijie Qiu, Yingcheng Wu, Shuya Li, Dingyan Wang, Zhuomin Zhou, Duo An, Yuhao Chen, Yu Li, Yongbo Wang, et al. Origene: A self-evolving virtual disease biologist automating therapeutic target discovery. *bioRxiv*, pp. 2025–06, 2025.

A APPENDIX

A.1 RAG DATABASE CONSTRUCTION

To construct the RAG dataset, we sourced 10,876 PDF papers in biology and chemistry from Open-DataLab [20]. We then converted these PDFs to plain text using MinerU [50] to ensure downstream readability and analyzability.

Because the raw corpus spans many topics, we designed a two-stage semantic filtering pipeline to focus the final corpus on biology- and chemistry-centric research.

We defined a set of positive keywords to capture target research areas, and in parallel, we curated negative keywords to exclude off-topic or tangential materials, as demonstrated in Figure A1.

Positive and Negative Keywords	
Positive Keywords	
<ul style="list-style-type: none">• Biology: <i>biology, DNA Replication, RNA Transcription, Protein Synthesis, Gene Editing, Viral Infection, Cell Signaling, Nucleic Acid Probes, Genomic Sequencing, Transgenic Technology, Immune Response, Biomarkers, Cell Culture, CRISPR Technology, Viral Vectors, RNA Interference, Gene Expression Regulation, Cell Differentiation, Metabolic Pathways, Apoptosis, Bioinformatics</i>• Chemistry: <i>chemistry, Organic Synthesis, Inorganic Chemistry, Catalysis, Polymer Chemistry, Spectroscopy, Crystallography, Chemical Kinetics, Thermodynamics, Electrochemistry, Quantum Chemistry</i>	
Negative Keywords	
<ul style="list-style-type: none">• Non-biology: <i>Cosmetics, Food Additives, Drug Advertising, Environmental Pollution, Ecological Balance, Medical Ethics, Social Sciences, Psychology, Nutrition, Educational Methods</i>• Non-academic chemistry: <i>Household Chemicals, Industrial Wastewater, Pesticide Residues, Fertilizer Application, Chemical Engineering Safety, Petrochemical Production</i>	

Figure A1: Positive and Negative Keywords.

This design concentrates positives on fundamental research fronts (e.g., gene editing, molecular signaling, organic synthesis, spectroscopy, thermodynamics) while negatives cover applied or peripheral themes (e.g., chemical production, pesticide residues, environmental pollution), improving separation of target papers from irrelevant content.

For filtering, we encoded each paper’s title and abstract with a pretrained Transformer and computed cosine similarities against the positive and negative keyword sets. Papers were retained only if

$$\cos(E_{\text{paper}}, E_{\text{positive}}) > 0.2, \quad \cos(E_{\text{paper}}, E_{\text{negative}}) < 0.1,$$

where E_{paper} denotes the vector representation of a paper’s title and abstract, and $E_{\text{positive}}/E_{\text{negative}}$ denote aggregate vectors of the positive/negative keyword sets. This step effectively removed content unrelated to biology and chemistry. The post-filter distribution is summarized in Table A1.

Table A1: Paper Classification Statistics by Domain (Side-by-Side)

Biology Category (n=2029)		% of Domain	Chemistry Category (n=359)		% of Domain
Molecular and Cell Biology (777)		38.39%	Organic Chemistry (172)		47.91%
Immunology and Microbiology (482)		23.76%	Physical Chemistry (71)		19.78%
Genetics, Genomics & Computation (411)		20.26%	Materials Chemistry (68)		18.94%
Neuroscience (205)		10.11%	Analytical Chemistry (37)		10.31%
Ecology and Evolution (149)		7.35%	Inorganic Chemistry (11)		3.06%

Overall Summary

Total Biology Papers: 2029 (100%)

Total Chemistry Papers: 359 (100%)

Total Papers: 2388 (100%)

After semantic filtering, we used a large language model (LLM) to extract structured text suitable for Retrieval-Augmented Generation (RAG). We designed a paper-specific prompt that guides the LLM to segment each paper into retrievable knowledge units (e.g., definitions, methods, experimental results, discussion) with consistent formatting across papers.

Prompt of RAG Bullet-Point Summarization

Role: You are an information synthesis assistant.

General Rules:

- Use ONLY the paper content provided below. No outside knowledge or invented facts.
- Do NOT include verbatim quotes, citations, or page references.
- The final output MUST be a single CSV code block with rows containing ONLY synthesized, self-contained bullet-point summaries for RAG.

Complete Paper Content:

```
{paper_content}
```

Objective: Read the entire paper content and internally construct self-contained knowledge paragraphs. Then derive standalone, self-contained bullet-point summaries from those paragraphs for retrieval-augmented generation (RAG). The intermediate knowledge paragraphs are an internal step and MUST NOT be printed in the final output.

Process:

- **Phase 1 Internal Knowledge Paragraphs (DO NOT OUTPUT):**
 - After reading the full content, synthesize a set of self-contained knowledge paragraphs.
 - Each paragraph must be strictly grounded in the provided text, define acronyms upon first use, include concrete details when available (tasks, datasets, sample sizes, metrics, effect sizes, confidence intervals, ablations, baselines, hyperparameters, assumptions, limitations), written in neutral third-person factual style, and able to stand alone without context from other paragraphs.
- **Phase 2 RAG Bullet-Point Summaries (FINAL OUTPUT ONLY):**
 - Produce around 3 bullet points in total.
 - Each bullet must be self-contained, concise (13 sentences), define acronyms upon first use, include concrete quantitative or methodological details when available, state scope/assumptions/limitations when given, and use neutral third-person factual style.

Output Format (CSV ONLY):

- Output EXACTLY ONE CSV code block and NOTHING ELSE.
- Header MUST be: `name, year, locator, topic, quote`
- For EACH bullet point, create ONE row with:
 - `name` = "SYNTHESIZED_POINT_SUMMARY"
 - `year` = N/A
 - `locator` = N/A
 - `topic` = N/A
 - `quote` = the bullets full self-contained text (escape quotes as needed; no line breaks inside a cell)
- Do NOT include the intermediate knowledge paragraphs in the output.
- Do NOT add extra columns or any prose outside the CSV block.

Begin: Output only the CSV code block.

Through this pipeline, we obtained a topic-focused, structurally consistent research corpus that provides high-quality knowledge support for downstream RAG systems.

A.2 AGENT PROMPT

A.2.1 REFINEMENT

The following shows the prompt we use in the HSR stage.

Prompt of Refinement

Assistant Prefix Prompt

```
<think>
Okay, I will answer user's problem by deep reasoning together
with writing python code in <code></code> format. I should
review and check the solution from student first with web
functions to identify errors if exist, then present my
solution and answer. For example
1. If I want to use the function of web_search(keywords),
will say:
keywords=...
results=web_search(keywords)
print(results)
2. If I want to use the function of web_parse(link, query),
will say:
link=...
query=...
results=web_parse(link, query)
print(results)
3. If I want to use the function of search_local_documents(query),
will say:
query="..."
documents=search_local_documents(query)
print(results)
4. If I want to do computation, I will write code for
accurate result:
a = 123
b = 456
print(a+b)
Now, let me analyze the user's question.
</think>
```

User Prompt

Problem

{query}

Anchor Solution

{anchor_solution}

Student 1's Solution

{reference_1}

Student 2's Solution

{reference_2}

Student 3's Solution

{reference_3}

Student 4's Solution

{reference_4}

Your Job

You should critically check the Anchor Solution to the problem, then correct it if needed and write your own answer.

1. Identify its weak points (missing reasoning steps, calculation errors, unclear logic, etc.).
2. You can refer to other students' solutions for targeted improvements relevant to those weak points.
3. Please note that other students' solutions may have errors. Please refer to the points worth learning and make improvements.
4. Apply repair strategies if needed:
 - Logic Completion (fill missing reasoning)
 - Numerical Correction (fix calculation errors)
 - Method Replacement (use a better method if needed)
 - Expression Refinement (clarify presentation)

Only use improvements that directly address anchors weak points. Avoid unnecessary information merging.

You can solve the problem with the help of feedback from a code executor. Every time you write a piece of code between `<code>` and `</code>`, the code inside will be executed. For example, when encountering numerical operations, you might write a piece of code to interpret the math problem into python code and print the final result in the code. Based on the reasoning process and the executor feedback, you could write code to help answering the question for multiple times (either for gaining new information or verifying). There are also several integrated functions that can be used to help you solve the problem. The available functions are:

1. `search_local_documents(query: str)` - this function takes a query string as input, and the output is a JSON string containing a list of relevant document snippets from a local, private knowledge base. This function should be your first choice for answering questions.
2. `web_search(keywords)` - this function takes keywords as input, which is a string, and the output is a string containing several web information. This function will call a web search engine to return the search results. This function is especially useful when answering knowledge-based questions.
3. `web_parse(link:str, query:str)` - this function takes the link and query as input, and the output is a string containing the answer to the query according to the content in this link. This function is useful when looking into detail information of a link.

Your workflow for solving the problem must follow these steps:

- Step 1: Local Document Search (Mandatory First Action): You must always begin by using `search_local_documents` to check for relevant information in the private knowledge base.
- Step 2: Evaluate and Supplement: After receiving results from `search_local_documents`, evaluate them carefully. Treat this information as a supplement to your background knowledge, not as absolute truth. This supplementary context may be incomplete or require further verification.
- Step 3: Web Search & Parse (Verification & Detail): After your initial local search, use `web_search` to find relevant web pages for verification or supplementation. If a specific link from the search results seems particularly useful, use

web_parse to extract detailed information from that page.

- You should not be overconfident in your knowledge and reasoning.
- Each time you write code put the code into `<code></code>` snippet. Put your final answer in `<answer></answer>` with `.`

The following shows the prompt we use in the QAIR stage.

A.2.2 QUALITY EVALUATOR

Prompt of Quality Evaluator

User Prompt

You are an expert evaluator. Your task is to evaluate the given solution for the problem from multiple perspectives.

Problem

{query}

Candidate Solution

{solution}

Evaluation Dimensions

1. Logical Reasonableness (0-5): Does the reasoning process follow valid logic?
2. Answer Correctness (0-5): Is the final answer correct and reasonable?
3. Explanation Completeness (0-5): Does the solution explain the reasoning clearly and completely?

Output Format

Return your answer strictly in JSON:

```
{
  "quality_scores": [float, float, float], // [logic, answer,
  explanation]
  "suggestion": "Provide an improvement suggestion for this
  solution that could help refine it in the next iteration."
}
```

The following shows the prompt we use in the RAG Monitor.

A.2.3 RAG MONITOR PROMPT

Prompt of RAG Monitor

Role: You are a helpful assistant.

Task: Analyze the following text and determine if responding to it accurately requires retrieving information from an external source.

Instructions:

- If you find any doubt or uncertainty about a concept or term in the text, consider it necessary to retrieve information (RAG).
- If retrieval is required, answer: yes.
- If no retrieval is required, answer: no.

Text:
{text}
Judgment:

The following shows the prompt we use in the RAG Querier.

A.2.4 RAG QUERIER PROMPT

Prompt of RAG Querier

Role: You are a helpful assistant.

Task: Generate a single, concise, and effective search query for retrieving the information required by the text below.

Instructions:

- Return **only the search query** itself.
- Do not include explanations, punctuation, quotation marks, or other text.
- The query should be direct and contain only the most essential keywords.

Text:
{text}
Search Query:

The following shows the prompt we use in the RAG Querier.

A.2.5 RAG INJECTOR PROMPT

Prompt of RAG Injector

Role & Core Objective: You are an information integration specialist. Your sole task is to process the provided RAG (Retrieval-Augmented Generation) output. Maximize the utilization of all relevant information to substantively support the reasoning, argumentation, or conclusions presented in the main text. Do not perform additional reasoning or generate new conclusions.

Content Integration Principles:

- **Comprehensive Extraction:** Extract all valuable information from the RAG outputs that enhances the logical depth, robustness, and persuasiveness of the main text's arguments.
- **Seamless Cohesion and Minimal Completion:** Maintain smooth contextual coherence and stylistic consistency. Perform minimal completion only if the main text ends mid-thought.
- **Neutral Representation:** Present all information objectively. Do not evaluate, question, or add subjective commentary.

Output Specifications:

- Output should follow the template: "{main text completion if necessary}_. Wait a minute, by searching information about {rag query}_, I found that {rag result}_. Now that I have more relevant information, I can continue my reasoning."
- Directly appendable to the end of the original main text.
- Do not include process summaries, headings, bullet points, or labels like "Supplement:".

Instruction Recap: Only select, filter, organize, and polish the RAG content. Do not perform external reasoning or add new information.

```
Main Text:
{text}

RAG Query:
{rag_query}

RAG Result:
{rag_result}
```

A.3 EVALUATION PROTOCOL AND ANSWER SCORING GUIDELINES

The o3-mini model was employed as an automatic judge to verify model-generated responses against the reference answers, following the official HLE Evaluation Prompts.

Prompt of Answer Evaluation

Role: You are an expert evaluator.

Task: Judge whether the following response to a question is correct or not based on the precise and unambiguous correct answer provided.

Question:
{question}

Response:
{response}

Correct Answer:
{correct_answer}

Evaluation Instructions:

- **extracted_final_answer:** Extract the final exact answer from the response. If there is no exact final answer, put 'None'.
- **reasoning:** Explain why the extracted_final_answer is correct or incorrect based on the correct answer. Focus only on differences between the response and correct answer. Do not comment on background, do not attempt to solve the problem, do not argue for any alternative answer.
- **correct:** Answer 'yes' if extracted_final_answer matches the correct answer (allow small margin for numerical problems). Answer 'no' otherwise (any inconsistency, ambiguity, or non-equivalency counts as 'no').
- **confidence:** Extract the confidence score from the response between 0% and 100%. If no score is available, put 100.

Output Format:

```
{
  "extracted_final_answer": "...",
  "reasoning": "...",
  "correct": "yes/no",
  "confidence": "...",
}
```

In Figure 8, the vertical and horizontal axes represent the scores assigned by the LLM for answer continuation, with output values ranging from 0 to 1. Below are the prompts used to assess the accuracy and consistency of the answers.

Prompt of Answer Accuracy Evaluation

You are a meticulous grader. Evaluate a set of solver responses (up to five) for one stage of a medical/biological question by comparing each responses FINAL + full RESP reasoning to the ground truth GT + official rationale R. Output a continuous accuracy in [0,1] for each response.

Inputs:

- Q: question stem (may or may not have multiple-choice options).
- GT: ground-truth answer. This can be a multiple-choice letter or a short text for free-response questions.
- R: official rationale (may be empty).
- FINAL[i]: the solver's extracted final answer from `< answer > ... < /answer >` (may be a letter or short text).
- RESP[i]: the solver's entire assistant message for response i in this stage.

How to grade (read carefully):

Grade one solver's response at a time, each solver's grading process should be independent, and should not rely on anything else except the solver's response, final answer, Q, R, and GT.

The grading process for one solver:

- Determine the solver's FINAL answer from FINAL[i]. If missing, infer only if RESP[i] makes the choice unambiguous; otherwise treat as unanswered.
- Compare against GT:
 - For multiple-choice questions, check if the letter matches GT (case-insensitive).
 - or free-response questions, check semantic equivalence to GT (normalize wording, allow synonyms or equivalent phrasing).
- Evaluate reasoning quality: Does RESP[i] align with R (key findings, mechanisms, exclusions)? Does it avoid contradictions, hallucinations, or irrelevant statements?
- Scoring recipe (simple, smooth, continuous); Use a continuous score reflecting BOTH aspects:
 - 0.94–1.00 → FINAL matches GT and RESP closely aligns with R with sound, non-contradictory reasoning.
 - 0.69-0.94 → FINAL matches GT but RESP shows minor gaps, superficiality, or small inconsistencies.
 - 0.34-0.69 → FINAL \neq GT, yet RESP shows substantial, partially-correct reasoning aligned with R (good differential, one key mistake).
 - 0.00-0.34 → FINAL \neq GT and RESP shows weak/mostly incorrect reasoning (some relevant bits).
 - 0.00 → Off-topic, unsupported, self-contradictory, or clearly wrong with no meaningful alignment to R.
- Penalize confidently wrong statements or contradictions; do not reward verbosity.

Return ONLY valid JSON in the following form:

```
{
  "items": [
    {
      "accuracy": <float in [0,1]>,
      "reason": "<=< 40 words justification>"
    },
    {
      "accuracy": ..., "reason": ...
    },
    ...
  ]
}
```

Now grade the following batch of responses:

- Q: *q*
- GT: *gt*
- R: *r*
- FINALS: *{final_items}*
- RESPONSES: *{resp_items}*

Prompt of Consistency Evaluation

You are an expert biomedical exam grader. Below are two independently generated solutions to the same question. Your task is to evaluate how consistent these two solutions are.

Instructions:

- Compare the reasoning processes, scientific logic, and final answers.
- Assign a consistency score from 0.00 to 1.00 (two decimal places):
 - 1.00 = Solutions are highly consistent (nearly identical reasoning and conclusion).
 - 0.00 = Solutions are completely inconsistent (different reasoning and conclusion).

Solution A:

{solution1}

Solution B:

{solution2}

Please provide your consistency score (e.g., 0.85):

A.4 EXTERNAL VALIDATION AND LIMITATIONS

Primary evaluation. As detailed above, our main results are scored automatically by o3-mini using the official HLE judging prompts and our continuous scoring rubric (Sec. A.3). No human expert adjudication is included in the reported metrics.

Risk of bias and robustness. Automatic judging ensures scalability and reproducibility but may introduce grader-specific biases and failure modes, especially for free-response rationales. To mitigate this concern and to support future replication, we pre-register a small-scale expert validation protocol focused on HLE free-response items:

- **Sampling.** Randomly sample $n=20$ items from HLE Bio/Chem (stratified by topic and difficulty), prioritizing free-response questions where judging is more nuanced than multiple choice.
- **Blinding.** Two independent domain experts (blinded to model identity and to each other’s scores) will grade each item using the exact same criteria as our o3-mini rubric (binary correctness and a continuous accuracy score in $[0, 1]$).
- **Outputs.** For each response, experts record: (i) extracted final answer, (ii) binary correctness, (iii) a continuous accuracy in $[0, 1]$ with ≤ 40 -word justification.
- **Agreement metrics.** We will report expert-expert agreement (percent agreement, Cohen’s κ for binary correctness; Pearson/Spearman for continuous accuracy) and expert-o3-mini agreement (macro-F1 for binary correctness; Pearson/Spearman correlations for continuous accuracy).
- **Release.** We will release the sampled IDs, anonymized expert score sheets, and scripts to recompute all agreement statistics in our artifact package.

Takeaway. While our main findings rely on automatic judging for scale and consistency, the above protocol provides a concrete path to independently verify fairness and robustness on the subset of free-response items where grader discretion matters most. We will include the full results of this expert validation in the camera-ready or artifact release.

A.5 RAG MONITOR HYPERPARAMETER SETTINGS

In our implementation of the RAG-enhanced reasoning agent, several key hyperparameters are used. Table A2 summarizes these hyperparameters and their functions.

The choice of query_top_k = 3 is motivated by our design of frequent and fine-grained monitoring. Each retrieval must be highly precise, since too many retrieved documents would unnecessarily lengthen the context, slow down reasoning, and introduce redundant or noisy information.

Hyperparameter	Value	Description
model	gpt-4.1-mini	LLM model used in RAG Monitor
query_top_k	3	Maximum number of retrieved documents for each query.
rag_chunk	512	Text chunk size for RAG monitoring.
rag_overlapping	128	Number of overlapping characters between consecutive chunks to maintain continuity.
max_rag	2	Maximum number of RAG insertions allowed in one reasoning step.
temperature	0.5	Controls generation diversity; higher values lead to more randomness.

Table A2: Main Hyperparameter Settings used in RAG Monitor.

The parameters `rag_chunk` and `rag_overlapping` control the monitoring frequency of the RAG module. A large `rag_chunk` would make detection too sparse, causing some uncertain reasoning fragments to miss external knowledge injection. The overlapping setting ensures continuity between consecutive windows and avoids missing potential triggers.

The parameter `max_rag` limits the maximum number of retrievals that can be inserted within one agent step. This prevents the monitor from triggering too frequently and ensures that the reasoning process remains stable and forward-moving.

In practice, the RAG monitor is triggered on average 3.64 times per 10,000 generated characters. Each trigger adds about 176.17 tokens of new context, resulting in an average of 641.25 additional tokens per 10,000 characters. Although this introduces extra tokens, it reduces the need for explicit tool calls, which significantly lowers the tool usage cost. As a result, the overall reasoning process requires fewer steps and consumes fewer tokens, as shown in Table 3.

A.6 ERROR CASE ANALYSIS

Here, we examine three representative failure modes of our model: reasoning-process errors, knowledge-application errors, and comprehension errors. In the subsections that follow, we present a real case for each and analyze how HSR and QAIR contributed to the failure.

A.6.1 CASE 1: REASONING PROCESS ERROR

HLE Question. Transgenic Arabidopsis lines constitutively expressing wheat proteins AKP1, RIB3, KIB1, and YKL23 were tested in three assays: (i) luminol-based ROS over 60 min to MAMPs (flagpep25–40, flagpep140–168, csp192–208), (ii) split-luciferase complementation in tobacco leaves, and (iii) GFP localization under water vs flagpep140–168. Choose the correct statement.

Answer Choices (A–H):

- A. AKP1 and RIB3 are redundant receptors for pepflag22.
- B. KIB1 is the receptor for flagpep25–40 and flagpep140–168 but not for csp192–208.
- **C. RIB3 is the coreceptor of AKP1; KIB1 acts downstream of RIB3.**
- D. All tested proteins are transmembrane proteins...
- E. YKL23 acts upstream of KIB1; RIB3 does not act upstream of KIB1.
- F. flagpep25–40 is the ligand for AKP1 and csp192–208 for YKL23.
- G. Tobacco lacks an endogenous homolog of AKP1.
- H. None of the above.

HSR (Hierarchical Solution Refinement)

Anchor s^* (initially correct): From the cross-modal evidence, the solver first forms the anchor “AKP1 requires RIB3 to sense flagpep140–168; KIB1 acts downstream” \Rightarrow favors C.

early pass supporting C:

```
"... the correct statement is choice C: 'RIB3 is the coreceptor
of AKP1;
KIB1 acts downstream of RIB3.'
- ROS: AKP1+RIB3 -> flagpep140-168 (2e6 RLUs), neither alone
  responds.
- Split-luc: AKP1<->RIB3 baseline suggests ligand-dependent
  complex;
  KIB1<->AKP1 and KIB1<->YKL23 are positive.
- GFP: KIB1 relocalizes under flagpep140-168; AKP1/RIB3/YKL23
  stay at PM."
```

HSR Error Note

Misweighting across modalities. HSR over-weighted split-luc magnitudes and under-weighted ligand dependence implied by ROS. **Missed consistency repair.** No reconciliation step to explain baseline AKP1↔RIB3 (no ligand) vs. positive ROS (with ligand).

Where HSR goes wrong (pivot to a faulty anchor): When a later refinement step over-weights split-luciferase magnitudes and under-weights ligand dependence, the anchor flips to E. Two faulty moves are visible in the refinement trace:

- **Fault 1 (magnitude ⇒ direction):** Interprets strong KIB1↔YKL23 (8e5 RLU) as *directional upstreamness* of YKL23 over KIB1, even though magnitude does not encode causal order.
- **Fault 2 (baseline ⇒ absence):** Treats AKP1↔RIB3 baseline (2e2 RLU) *without ligand* as evidence against co-reception, ignoring the ROS gain-of-function with AKP1+RIB3 under flagpep140-168 (a classic ligand-dependent complex pattern).

refinement pivot toward E:

```
"... search_local_documents timed out. Proceed from assays.
KIB1<->YKL23 is strong (8e5), AKP1<->RIB3 is baseline (2e2),
so YKL23 likely acts upstream of KIB1 and RIB3 does not.
Final choice: E."
```

HSR diagnosis: The error is *reasoning process*, not missing knowledge. All requisite facts (ROS synergy for AKP1+RIB3 at 140-168; KIB1 relocalization; split-luc positives with KIB1) are available, but the refinement applies invalid inference rules that overturn the initially correct anchor C.

QAIR (Quality-Aware Iterative Review)

Checks logged as performed vs. missed:

```
Performed:
- Parse ROS matrix (AKP1+RIB3 -> 140-168; YKL23 -> csp192-208):
  OK
- Parse split-luc matrix (KIB1<->AKP1, KIB1<->YKL23 positive;
  AKP1<->RIB3 baseline): OK
- Consistency of the "E" narrative with split-luc magnitudes: OK

Missed:
- Cross-modal reconciliation: ligand-dependent complexes can
  yield
  baseline split-luc (no ligand) yet positive ROS (with ligand).
- Directionality audit: interaction magnitude != causal
  upstreamness.
- Sanity link: GFP relocalization of KIB1 implies downstream
  role,
  which conflicts with "YKL23 upstream of KIB1" narrative.
```

QAIR Error Note

Missed mandatory audits. QAIR should have enforced:

- Cross-modal reconciliation requires an explanation for baseline split-luc vs. positive ROS under ligand.
- Directionality audit disallow inferring causal order from interaction magnitude alone.
- Downstream sanity link KIB1s relocation supports a downstream role; flag conflict with the YKL23 upstream of KIB1 story.

Skipping these allowed a self-consistent but **incorrect** E narrative to pass.

Observed plateau: QAIR accepts internal consistency of the E narrative without enforcing cross-modal reconciliation, so the faulty anchor persists.

finalization kept by QAIR:

```
"... Based on strong KIB1<->YKL23 luminescence and no
      AKP1<->RIB3 signal,
      YKL23 acts upstream of KIB1, and RIB3 does not act upstream of
      KIB1.
<answer>E</answer>"
```

A.6.2 CASE 2: KNOWLEDGE APPLICATION ERROR

HLE Question. A university field trip samples bats on an island for one month (methodology assumed valid). The student computes Simpson's diversity index using the formula $D = 1 - N(N-1)/\sum n(n-1)$ and obtains $D = 0$. Which statement best describes this result?

Answer Choices:

- **A. Mathematically and ecologically valid**
- B. Mathematically inconclusive with the index value provided
- C. Not mathematically valid, but ecologically valid
- D. Mathematically valid, but not ecologically valid
- E. Not mathematically or ecologically valid

HSR (Hierarchical Solution Refinement)

Initial anchor (as formed): Accept the problems formula exactly as stated, derive what $D = 0$ implies under that formula, then judge mathematical vs. ecological validity.

problem framing and anchor start:

```
"... the standard Simpson's diversity index is either (1 -
      lambda) or (1/lambda)
      where lambda = sum n_i(n_i - 1)/[N(N-1)]. The formula given in
      the problem,
      D = 1 - N(N-1)/sum n(n-1), is not standard. However, for the
      purpose of this
      problem, we must work with the formula as stated.

      The student obtained a value of 0, which occurs when sum n(n-1)
      = N(N-1) ..."
```

What HSR should have applied (correct knowledge use):

- *Ecological validity is evaluated against the observed community in the stated sampling frame* (the one-month survey), not against lifetime site anecdotes.
- Given the solver already decided to use the provided formula as stated, $D = 0$ is mathematically valid and, if the months sample indeed shows one species, *ecologically valid for that sample* \Rightarrow A.

HSR Error Note

Misapplied knowledge at refinement. Instead of auditing ecological validity within the *sampling frame*, HSR imported out-of-frame site priors (known island diversity), which **overrode** the sample-level conclusion. **Missed consistency repair.** After explicitly deciding to work with the formula as stated, HSR later allowed a pivot to wrong formula \Rightarrow option 4, without a reconciliation step.

What actually happened in HSR (knowledge misapplication): The refinement step imported site-level prior knowledge (known island diversity) to overrule the sample-level ecological judgment and flipped away from A.

knowledge misapplication trace:

```
"- Ecological validity: Ecologically, it is invalid because it
  contradicts the
  known diversity of the island, as multiple species are known to
  exist."
```

```
"The student chose D, which is option 3."
```

refinement concluding to option 4 in this run:

```
"... using a wrong formula makes it mathematically invalid.
Thus, the correct answer is option 4: Not mathematically or
ecologically valid.
<answer>E</answer>"
```

HSR diagnosis: The error is *knowledge application*. The solver had all needed facts (including the decision to use the given formula and the implication of $D = 0$) but applied ecological knowledge at the wrong level (site history rather than the sampled community), causing the anchor to settle on D or E instead of A.

QAIR (Quality-Aware Iterative Review)

Checks recorded as performed vs. missed (from the run text):

```
Performed:
- Algebra under the given D-formula:  $D = 0 \Leftrightarrow \sum n(n-1) = N(N-1)$  (OK).
- Consistency of "mathematically valid" under the accepted
  (given) formula (OK).

Missed:
- Ecological validity audit constrained to the stated sampling
  frame
  (evaluate representativeness of the one-month sample, not
  lifetime site knowledge).
- Consistency check: if the month legitimately observed a
  single-species sample,
  then both mathematical and ecological validity hold  $\Rightarrow$  Choice
  A.
```

QAIR Error Note

Missed mandatory audits. QAIR should have enforced:

- Sampling-frame ecological audit - judge ecological validity only within the months survey.
- Formula-consistency audit - after use the formula as stated, reject later pivots to wrong formula unless reconciled.
- Gold-aligned sanity check - if the accepted sample contains one species, then *both* mathematical and ecological validity hold \Rightarrow A.

Skipping these allowed a self-consistent but **incorrect** narrative (ecologically invalid due to island history) to pass.

Observed plateau: QAIR validated internal consistency of the ecologically invalid due to island history narrative and did not enforce a sampling-frame ecological audit, so the faulty anchor persisted.

finalization kept by QAIR in this run:

```
"... Ecologically ... known diversity on the island ... making
the result
ecologically invalid. Thus ... corresponds to option 3."
<answer>4</answer>
```

A.6.3 CASE 3: COMPREHENSION ERROR

HLE Question. A university field trip samples bats on an island for one month (methodology assumed valid). The student computes Simpson's diversity index using the formula $D = 1 - N(N-1)/\sum n(n-1)$ and obtains $D = 0$. Which statement best describes this result?

Options:

- **A. Mathematically and ecologically valid**
- B. Mathematically inconclusive with the index value provided
- C. Not mathematically valid, but ecologically valid
- D. Mathematically valid, but not ecologically valid
- E. Not mathematically or ecologically valid

HSR (Hierarchical Solution Refinement)

Anchor s* (as formed by the solver): correct mechanism up to the enal stage (thermolysis of the sulfoxide \rightarrow vinyl ether \rightarrow [3,3]-Claisen \rightarrow unsaturated aldehyde).

excerpt from the run (mechanistic anchor):

```
"... thermal elimination at 180 C gives the vinyl ether
CH2=CH-O-C(CH3)2-CH=CH2,
which undergoes a [3,3]-sigmatropic Claisen rearrangement to an
aldehyde ..."
```

Where HSR should have repaired comprehension (nomenclature layer): For aldehydes, the parent chain must (i) include the carbonyl carbon as C1 and (ii) maximize chain length while assigning the lowest locants jointly to C=O and the C=C. Under the rearranged connectivity, the correct parent is *hex*, absorbing one methyl into the main chain; the double bond is at C4 and the remaining methyl is at C5, yielding *5-methylhex-4-enal* (Gold).

HSR Error Note

Missed comprehension repair. HSR failed to:

- apply the aldehyde *parent-chain rule* (chain must include C=O and be maximized);
- apply the *lowest-locant rule* for the C=C within that parent;
- re-evaluate *pent-** vs. *hex-** after the [3,3]-shift mapping.

Result: the naming anchor should have flipped to **5-methylhex-4-enal**, but did not.

What actually happened in HSR (missed repair; wrong anchor kept): The refinement layer accepted a *pent*-based chain and locked the name accordingly.

excerpts from the run (mis-naming kept by refinement):

```
"The IUPAC name is derived as follows:
- The longest carbon chain containing the aldehyde group is five
  carbons (pentanal).
- The double bond is between carbons 4 and 5 (pent-4-enal).
- Two methyl groups are attached to carbon 3 (3,3-dimethyl).
Thus, the correct name is 3,3-dimethylpent-4-enal.

<answer>
\boxed{3,3-dimethylpent-4-enal}
</answer>"
```

HSR diagnosis: The failure is *comprehension* of IUPAC chain selection rules (parent-chain identification when both a C=O and an alkene must be included), not mechanism recall. HSR improved mechanistic clarity but did not apply a naming-level repair to flip from *pent-** to the *hex-** parent required by the Gold answer.

QAIR (Quality-Aware Iterative Review)

Checks recorded (as reflected in the run text):

- Mechanistic plausibility (elimination → vinyl ether → Claisen): PASSED
- Role of NaHCO₃ as neutralizing base (sulfenic acid): PASSED
- Internal consistency of proposed names vs. drawn skeleton: PASSED
- IUPAC audit: parent-chain selection and lowest-locant C=C (REQUIRED): SKIPPED

QAIR Error Note

Missed mandatory audit. QAIR should have enforced:

- Parent-chain audit (aldehyde rule): chain includes C=O and is maximized;
 - Lowest-locant audit (C=C) within that parent chain;
 - [3, 3] - mapping check to determine which branch becomes part of the main chain.
- Skipping these allowed a self-consistent but **wrong** *pent-** narrative to pass.

Observed plateau: QAIR converged on a self-consistent *pent*-chain narrative and terminated without running the naming audit that would force re-evaluation of the parent chain under aldehyde rules.

Conclusion kept by QAIR:

```
"... The major product is 4,4-dimethylpent-5-enal ...
<answer> \boxed{4,4-dimethylpent-5-enal} </answer>"
```

A.7 ADDITIONAL BENCHMARK RESULTS

A.8 PSEUDO-CODE

A.9 USAGE OF LANGUAGE MODELS

We utilized a large language model (LLM) to aid in the preparation of this manuscript. Its use was limited to editorial tasks, including proofreading for typographical errors, correcting grammar, and improving the clarity and readability of the text.

Table A3: Benchmark comparison on HLE Bio/Chem (149 problems; o3-mini judge)

Model	Acc (%)
<i>LLMs</i>	
DeepSeek V3.1 (Non-Think)	6.71
Deekseek R1	10.74
Qwen3 235B A22B	15.38
<i>LLM with Tools</i>	
Deekseek R1 with Browsing	16.82
DeepSeek V3.1 with Browsing	11.21
Doubao with Browsing	11.21
<i>Agents</i>	
Kimi Researcher	9.35

Algorithm 1 Eigen-1: High-level Workflow

Require: Query q , config \mathcal{C} (LLM & retriever), #proposers K (e.g., 5), QAIR threshold τ , max rounds T_{\max}
Ensure: Final solution s^*

```
1: Init: set up LLM, RETRIEVER, and tool endpoints from  $\mathcal{C}$ 
2:
   Proposer generates initial solutions
3: for all  $i \in \{1, \dots, K\}$  in parallel do
4:    $S[i] \leftarrow \text{GENERATE}(q)$  ▷ initial solution generation
5: end for
6:
   Local correction (optional, per-candidate)
7: for all  $i \in \{1, \dots, K\}$  in parallel do
8:    $C[i] \leftarrow \text{CORRECTOR}(S[i])$  ▷ targeted fixes without cross-solution access
9: end for
10:
   Hierarchical Solution Refinement (HSR)
11:  $R \leftarrow \emptyset$ 
12: for  $a \in \{1, \dots, K\}$  do ▷ rotate anchors
13:    $A \leftarrow C[a]$ ,  $Ref \leftarrow C \setminus \{C[a]\}$ 
14:    $R[a] \leftarrow \text{REFINE}(A, Ref)$  ▷ apply peer-informed repairs: logic, numeric, method, expression
15: end for
16:
   Quality-Aware Iterative Reasoning (QAIR)
17:  $t \leftarrow 0$ ,  $P \leftarrow R$ 
18: while  $t < T_{\max}$  do
19:   (parallel) for each  $s \in P$ :  $(q_{\text{logic}}, q_{\text{ans}}, q_{\text{exp}}, \text{suggestion}) \leftarrow \text{EVALUATOR}(s)$ 
20:    $\text{score}(s) \leftarrow 0.2 \cdot q_{\text{logic}} + 0.6 \cdot q_{\text{ans}} + 0.2 \cdot q_{\text{exp}}$ 
21:    $Pass \leftarrow \{s \in P \mid \text{score}(s) \geq \tau\}$ ;  $Fail \leftarrow P \setminus Pass$ 
22:   if  $Fail = \emptyset$  then break
23:   end if
24:   (parallel) for each  $s \in Fail$ :  $\tilde{s} \leftarrow \text{CORRECTOR}(s, \text{suggestion})$ 
25:    $P \leftarrow Pass \cup \{\tilde{s} \mid s \in Fail\}$ ;  $t \leftarrow t + 1$ 
26: end while
27:
   Rank & select
28:  $s^* \leftarrow \text{RANKER.SELECT}(P)$  ▷ e.g., composite score or pairwise compare
29: return  $s^*$ 
```

Subroutines used in all LLM generation process

```
30: function MONITOR-BASED RAG( $q$ )
31:    $ctx \leftarrow \text{INITCONTEXT}(q)$ 
32:   while not DONE( $ctx$ ) do
33:      $ctx \leftarrow \text{LLM.NEXT}(ctx)$ 
34:     if MONITOR( $ctx$ ) = 1 then ▷ detect uncertainty/insufficiency on-stream
35:        $qry \leftarrow \text{QUERIER}(ctx)$  ▷ minimal, targeted keywords
36:        $docs \leftarrow \text{RETRIEVER}(qry)$ 
37:        $ctx \leftarrow \text{INJECTOR}(ctx, docs)$  ▷ compress & integrate evidence seamlessly
38:     end if
39:   end while
40:   return TRACEToSOLUTION( $ctx$ )
41: end function
```
