LLM-Assisted Plasma Simulation Code Automation: Draft 3

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Abstract

Contents

1. Introduction

1.1 Numerical simulations of fusion plasmas (big picture of fusion research)

Modern nuclear-fusion research relies heavily on **gyrokinetic simulation**, which reduces the full 6D kinetic plasma problem into a more tractable form while preserving key microturbulence physics. This shift enabled first-principles turbulence studies and transport predictions that are difficult to obtain experimentally, and it is now routine to use large gyrokinetic codes for tokamak/stellarator turbulence and validation studies (e.g., GENE, GS2, GTC, GKV and related validation work). (MPG.PuRe)

Fusion devices are large-scale, and plasma phenomena span wide spatiotemporal scales that cannot be fully measured. Numerical simulation is therefore essential for device design, operation scenarios, and understanding plasma physics. To cover wide scales and incorporate detailed physics, simulation codes are large and interdependent; advances in computing have improved reproducibility but raised the barrier to new contributors.

However, **gyrokinetic simulation software is hard to extend**:

- **Large, interdependent codebases**: physics modules (e.g., collisions, electromagnetic terms, geometry, diagnostics) are spread across many files and abstraction layers.
- **High cost per new feature**: adding a small physics change (e.g., a collision term, equilibrium interface, or diagnostic) often requires edits across data structures, solvers, I/O, tests, and documentation.
- **High onboarding cost**: new contributors must learn both the physics and the code architecture before making safe changes.

Large Language Models (LLMs) are becoming practical tools for software development and scientific workflows, especially when paired with **external knowledge, tools, and structured agent pipelines**. This motivates building an LLM system that helps fusion researchers understand unfamiliar codebases and implement changes more reliably.

1.2 Ultimate research goal: problem solving with LLMs (knowledge pool and retrieval learning are key)

The long-term goal is to build an LLM inference system that improves reasoning and conversation with plasma researchers:

1. Improve reasoning by providing the system with source code and relevant papers/documents.
2. Improve conversation by capturing expert knowledge during interactions.
3. Reuse that knowledge in later sessions to solve new problems more effectively.

1.3 Bachelor thesis goal: error removal (subject to change)

For this bachelor thesis, the near-term goal is error removal and evaluation of an LLM-based system:

- Create a dataset from a fusion simulation codebase.
- Train the system and evaluate its performance on repair tasks.
- Refine the workflow and knowledge pool based on observed failure modes.

1.4 Organization of the thesis

The paper is organized as follows:

- Section 2 reviews LLM research and the SEIMEI/RMSearch framework.
- Section 3.2 describes dataset construction with (problem, code, answer) tuples.
- Section 3.3 presents the inference pipeline for codebase analysis and patch generation.
- Section 3.4 explains knowledge creation for problem solving.

- Sections 3.5 to 3.7 describe knowledge search training and evaluation.
- Sections 4 to 6 present experiments, discussion, and conclusions.

2. Large Language Model

2.1 Current Development on Large Language Models

The last several years produced a “stack” of advances that (together) explain why modern LLM systems can help with non-trivial scientific coding.

(1) Transformers

Most modern LLMs are based on the **Transformer**, which replaces recurrence with **self-attention**. Intuitively:

- In an RNN, information must flow step-by-step through time.
- In a Transformer, each token can “look at” other tokens directly (through attention), which enables **parallel training** and better long-range dependency handling.

This architecture made it feasible to scale training to very large datasets and models while keeping optimization stable. (arXiv)

(2) Scaling laws (and compute-optimal training)

Scaling law work observed that model loss often follows **smooth power-law trends** as you increase model size, data size, and compute—meaning progress can be predicted and engineered. (arXiv) Later work showed that, under a fixed compute budget, many LLMs were “undertrained” on too few tokens, motivating **compute-optimal** training strategies (often summarized via the “Chinchilla” perspective). (arXiv)

Why this matters for scientific coding: scaling isn’t just “bigger is better”—it also teaches how to spend compute efficiently, which becomes important when we later discuss RL-based post-training costs.

(3) InstructGPT / RLHF (often PPO-based)

Base LLMs are trained to predict the next token, not to follow instructions. InstructGPT-style pipelines added a practical recipe:

1. Collect **human-written demonstrations** (supervised fine-tuning).
2. Collect **human preference rankings** over model outputs.
3. Train a **reward model** to predict those preferences.
4. Optimize the policy using RL (often **PPO**) to improve reward while limiting drift from the base model.

This line of work improved instruction-following and user preference alignment—even showing cases where a much smaller aligned model is preferred to a much larger base model. (arXiv) The broader “learning from preferences” setup is also well-established in RL. (arXiv)

(4) DPO (Direct Preference Optimization)

DPO reframes preference optimization as a **simple classification-like objective** that can match RLHF-style goals (reward maximization with KL constraint) without running full RL rollouts. Practically, that means:

- No explicit reward model is required at training time (it's "implicit").
- Training looks closer to supervised fine-tuning, often simplifying stability and reducing engineering overhead.

This matters for us because we want a training loop that is realistic for academic GPU budgets. (arXiv)

(5) DeepSeek-R1-style reasoning-focused post-training

Recent reasoning-focused model releases and reports (e.g., DeepSeek-R1) highlight renewed emphasis on **reinforcement learning / preference optimization** as a path to stronger reasoning behavior, often combined with careful data and evaluation design. (arXiv)

For our paper's narrative, the key point is not "one model is best," but that the field trend increasingly treats **post-training (preferences, RL, or RL-free variants like DPO)** as a major lever for reasoning and reliability.

(6) Test-time compute (inference-time search)

Even without changing model weights, you can often improve reasoning by spending **more computation at inference time**. Common patterns:

- **Chain-of-thought prompting**: ask the model to write intermediate steps. (OpenReview)
- **Self-consistency**: sample multiple reasoning traces and pick the majority-consistent answer. (Astrophysics Data System)
- **Tree of Thoughts (ToT)**: explicitly search a tree of partial solutions, backtrack, and evaluate branches. (OpenReview)

A simple analogy: instead of trusting the first draft, you ask the model to generate multiple candidate "proof attempts," then select or refine the best. This "test-time search" theme is directly relevant to agentic coding pipelines, where we can try multiple patch candidates and score them.

Why RL can help, and why it can be expensive

Empirically, preference/RL-style post-training often improves **instruction following** and sometimes **reasoning benchmark performance**, but it can be resource-intensive because it requires generating many samples (rollouts) and performing multiple optimization steps (e.g., PPO). (arXiv) This motivates exploring **RL-free** (or "more supervised-like") alternatives such as DPO where appropriate. (arXiv)

2.2 SEIMEI

In this work we use **SEIMEI**, an open-source library that orchestrates LLM-based inference as a **search-integrated agent pipeline**. Conceptually, SEIMEI is designed for tasks requiring domain-specific knowledge and reasoning. SEIMEI realizes this by reinforcement-learning on search model which integrates agents and knowledge. (GitHub)

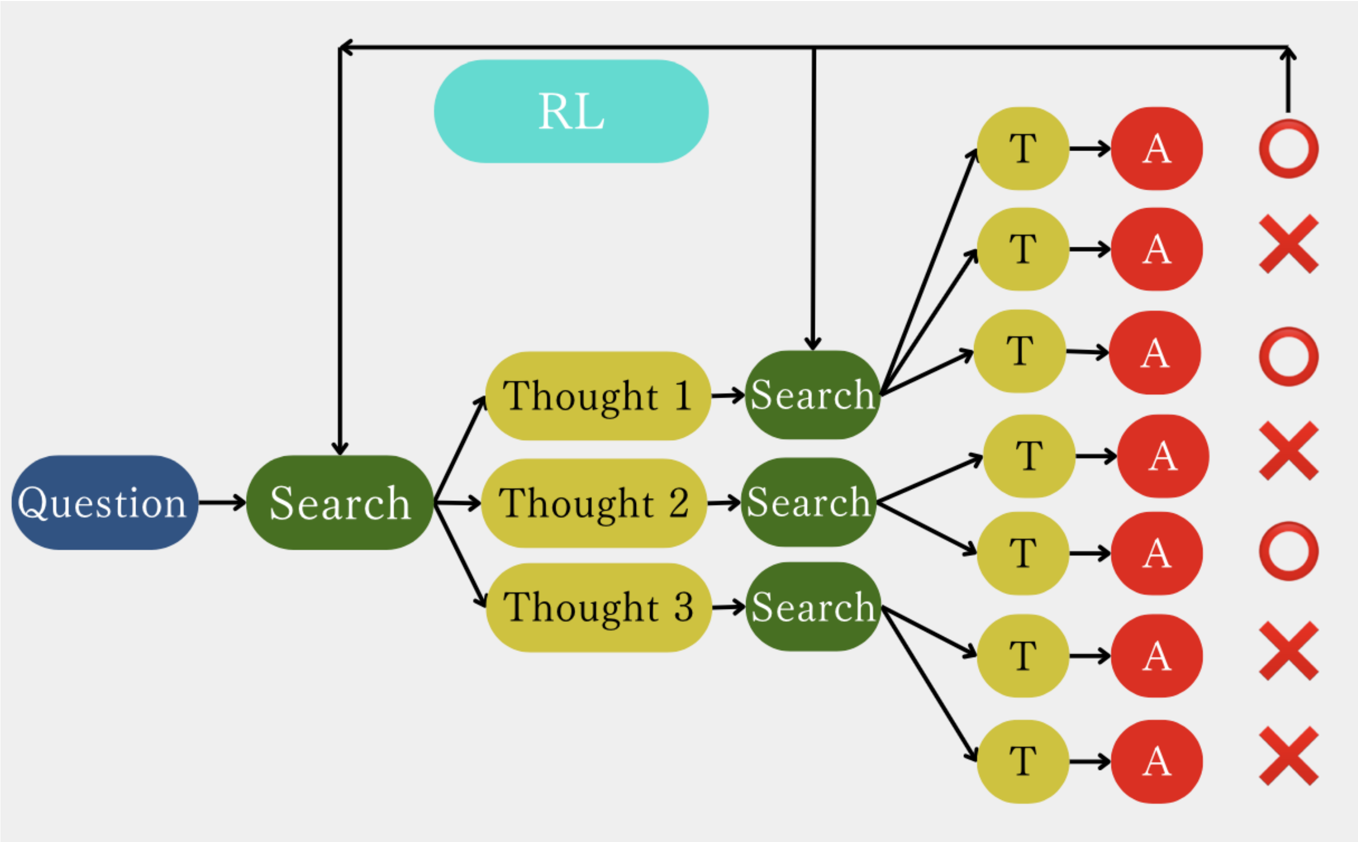

Figure | SEIMEI's inference and learning pipeline. Reinforcement-learning on search model improves the model reasoning path through guiding its thought.

Key idea (plainly): instead of training LLM on next token prediction task, SEIMEI **trains search model to guide inference**. This feature has the following advantage over the previous method.

1. Training search model doesn't break the core inference LLM, which prevents core inference collapsion (!need to add continuous learning citation).
2. Adapting search model to one domain requires much less calculation cost than training next-token-generation LLM.

Search has been a key technology for knowledge expansion. Search-engine has connected numerous amount of documents created by citizens and enabled human-beings to enhance the whole search-engine system by adding their own knowledge. This flexiblity to adding knowledge is key to expanding knowledge for an AI system. SEIMEI has a potential to become a new AI system - search model integrates not only simple knowledge but also how to think - beyond current workflow agent paradigm.

2.3 RMSearch

SEIMEI’s routing and knowledge selection use **RMSearch**, a reward-model-style search/reranking component. RMSearch retrieves and prioritizes helpful snippets (knowledge, prior solutions, docs, heuristics) that augment the LLM’s next step. (GitHub)

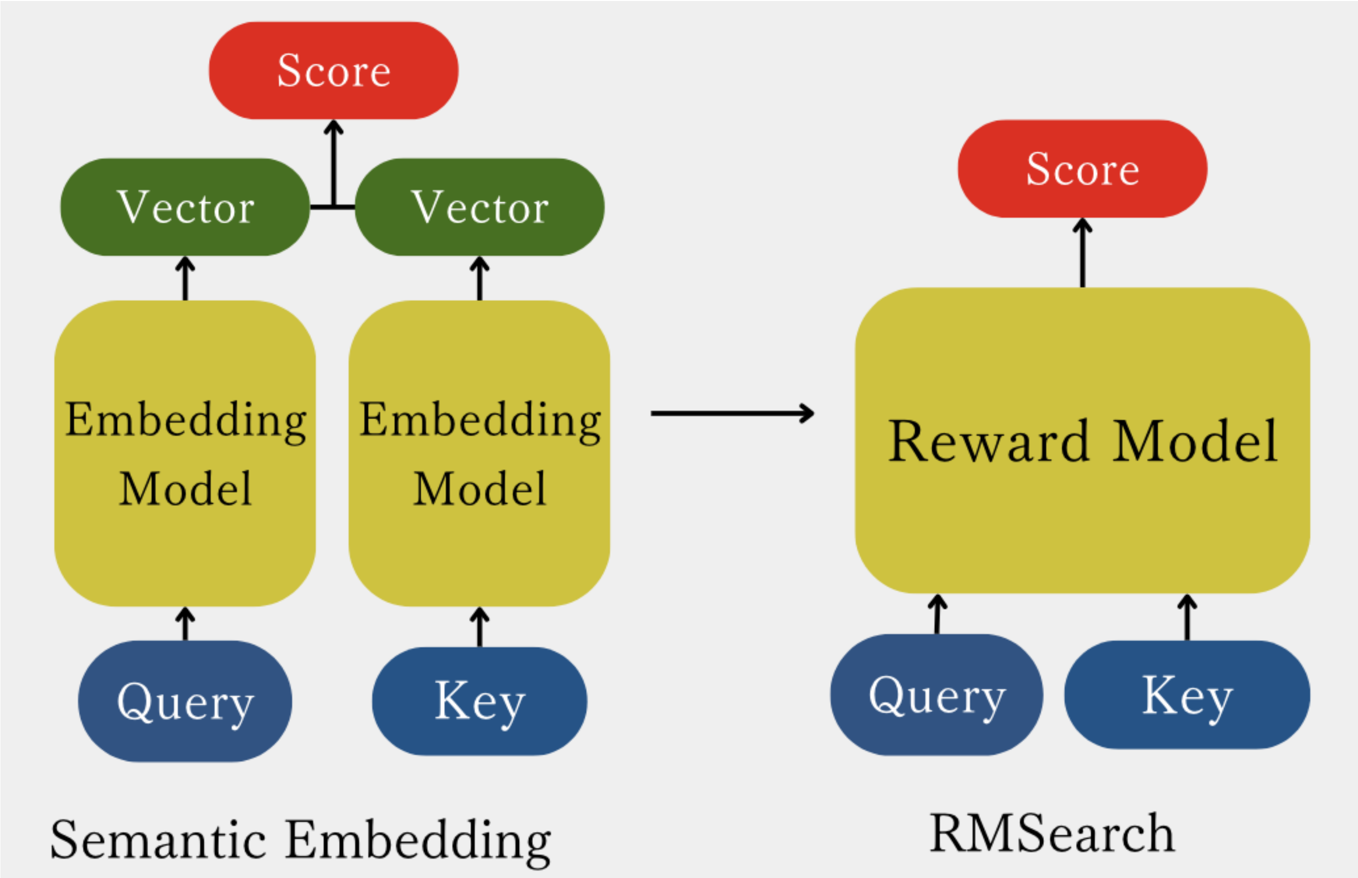

Figure | Model architecture difference between conventional vector search model and RMSearch.

Architecturally, RMSearch is closest to a **reranker**: given a query and candidate texts, it scores query–candidate relevance (often with a cross-encoder-style setup). This aligns with a long line of reranking research, including BERT-style rerankers and efficient interaction models. (arXiv)

The practical difference is the retrieval pipeline. In many systems, a dense retriever first returns a top-k set (e.g., 100), and a reranker then reorders that shortlist to select the final few. RMSearch instead scores candidates directly with the reward model, so relevance is computed with the same signal used for selection rather than as a separate post-processing stage.

RMSearch (reranking) matters especially in domain-specific search, where generic embedding similarity can miss task-relevant signals. A dense retriever compresses text into vectors, while a reward model learns to score relevance directly from paired query-candidate text. This makes RMSearch easier to adapt to a specific domain with preference data. (GitHub)

2.4 Goal of our research

We aim to improve LLM-assisted **plasma simulation code writing/editing** using SEIMEI + RMSearch, with an emphasis on gyrokinetic code (GKV). Our plan:

1. Build an inference system using SEIMEI.
2. Generate a dataset from a real gyrokinetic codebase.
3. Generate a **knowledge pool** by solving/repairing tasks (and extracting reusable lessons).
4. Train RMSearch (reranker-style) over that knowledge pool using preference-style data (DPO).
5. Measure whether the knowledge pool + trained RMSearch improves code-repair accuracy in the same domain.

(Experiments/results are not included in this baseline draft, per your request.)

2.5 Related Research

Below are the main research threads we build on; this section is intentionally plain and cross-disciplinary.

Retrieval-Augmented Generation (RAG)

RAG methods attach an external memory (documents, snippets, code, papers) to an LLM so it can **retrieve** relevant context rather than relying only on parameters. The core motivation is modularity:

- You can update knowledge by updating the corpus/index, without retraining the whole model.
- You can attach provenance ("this answer used these sources").

Classic RAG work combines a neural retriever with a generator for knowledge-intensive tasks. (arXiv) Related lines include retrieval during pretraining (REALM) (arXiv) and retrieval-enhanced generation at very large scale (RETRO). (arXiv) Dense retrieval also became a standard baseline for open-domain QA and retrieval pipelines. (arXiv)

Why it matters here: codebases are "documents." A fusion code repository contains the ground truth for function contracts, data layouts, and physics assumptions. RAG-style grounding reduces hallucinated edits.

AI agents (tool use, browsing, iterative editing)

Modern "LLM agents" combine a language model with tools and iterative control:

- Tool use learned or prompted (e.g., Toolformer). (arXiv)
- Modular architectures mixing LMs with specialized components (MRKL). (arXiv)
- Reason+act prompting patterns (ReAct), useful for multi-step tasks. (GitHub)
- Web/tool-assisted answering and reference collection (WebGPT), relevant for grounded reasoning workflows. (arXiv)
- Software-engineering agents with repository navigation and editing interfaces (SWE-agent). (arXiv)

Agent frameworks in practice often emphasize *interfaces* (file editing, running checks, browsing) rather than only better prompts—this aligns with our SEIMEI design goal of structured code repair. (arXiv)

DSPy (automatic pipeline improvement from evaluation)

DSPy proposes a programming model where you declare an LLM pipeline, define a metric, and let a compiler-like optimizer improve prompts/modules using data. (arXiv)

Connection to our goal: we also want an "evaluation-driven improvement loop," but focused on (a) code repair tasks, and (b) improving retrieval/reranking (RMSearch) and knowledge pools that feed the pipeline.

Reranker models (relevance scoring)

Rerankers are a standard IR technique: a fast retriever gets candidates; a stronger model reorders them. BERT reranking (monoBERT) demonstrated large gains in passage ranking. (arXiv) ColBERT provides an efficiency–quality tradeoff via late interaction. (arXiv)

Connection to our work: RMSearch plays the reranker role for “which knowledge or context should the agent use next,” which becomes crucial in specialized domains like gyrokinetics.

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3. Approach

3.1 Overview

Our approach is an end-to-end loop that turns a real fusion codebase into (1) code-repair tasks, (2) an agentic inference pipeline, and (3) training data for a domain-adapted reranker (RMSearch):

1. **Dataset creation**: intentionally break code, then create a question that asks for a repair.
2. **Inference pipeline**: given (question, broken code), generate a patch/repair candidate.
3. **Scoring**: evaluate candidate repairs (static checks, diff quality, possibly tests/compilation when available).
4. **Knowledge generation**: collect reusable “lessons” from successful (and failed) repairs.
5. **RMSearch dataset construction**: create preference pairs over candidate knowledge/context and/or candidate repairs.
6. **Train RMSearch** (DPO-style preference optimization).
7. **Evaluate**: run the inference pipeline again, now routed/augmented by trained RMSearch.

This is designed to be feasible without full RLHF infrastructure, while still leveraging preference-style learning.

3.2 Dataset Creation

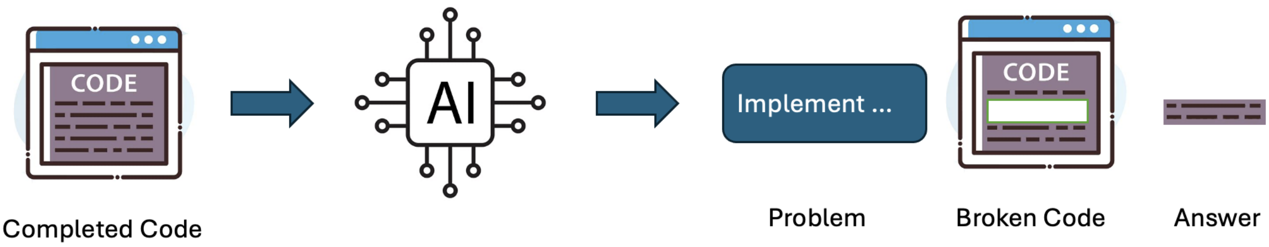

Figure | Dataset generation pipeline. Make LLM intentianlly break complete code and generate problem related to repairing the code snippet.

Target repository: we use the open gyrokinetic Vlasov simulation code **GKV (gkvp)** as the source code to generate dataset from. (GitHub)

Task type (plain description): “repair the code so it matches the original intended physics-aware behavior.”

Concretely, for a given file:

1. An LLM selects **which line(s) to break**, with the constraint that the deletion should affect **core physics logic** (not only comments or trivial formatting).
2. The pipeline generates:

   - a **patch** that removes important lines,
   - a **question** describing the observed failure or missing behavior ("restore the missing computation / boundary condition / term") and ask LLM to fix the issue.
3. An LLM debug patches: a patch often is not valid when it is applied to the file, so an LLM trys to modify the patch file from the error message for several times in this stage. If some patches still get error after this process, they are removed.

Why "break-and-repair" is useful:

- **Correctness:** It provides a clean answer patch because the correct fix is known. LLM can easily check if the LLM output is correct by comparing it with the original code.
- **Scalability:** This method only requires complete code and LLM request. It can be easily scaled to other complete code about plasma physics or even to other fields.
- **Realistic:** It creates physics-centered code edition problem which researchers often encounter in small code addition or fix related to plasma equations.

3.3 Inference Pipeline

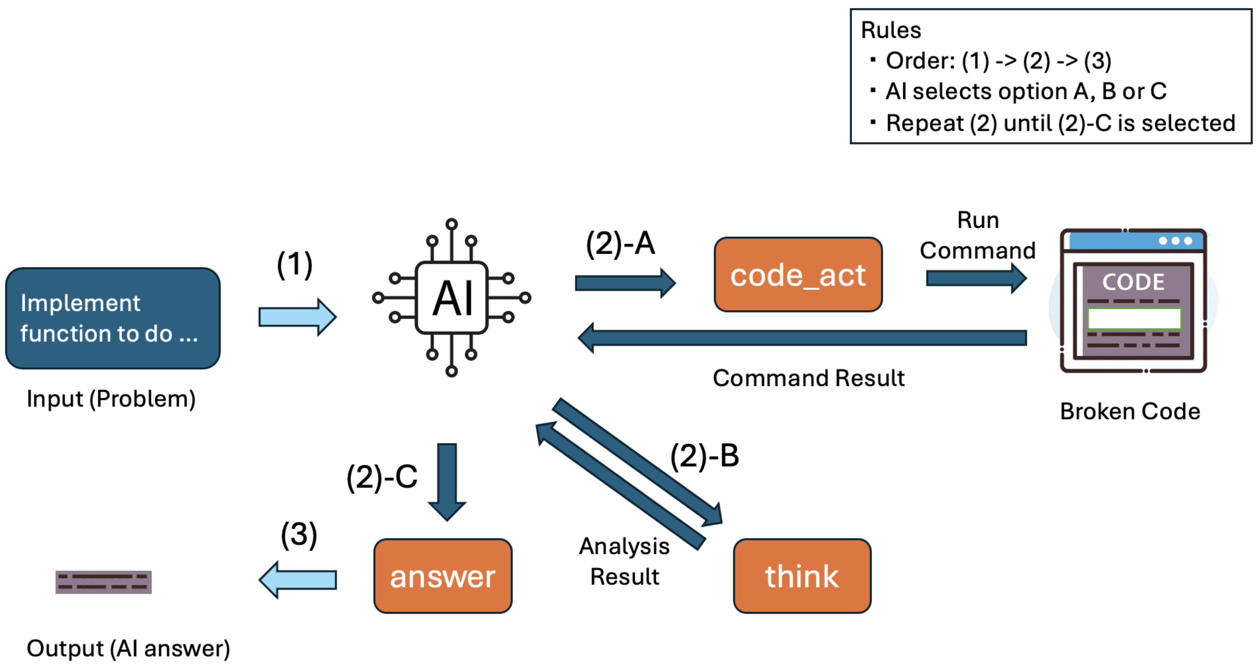

Figure | Normal approach to access code base and solve problem.

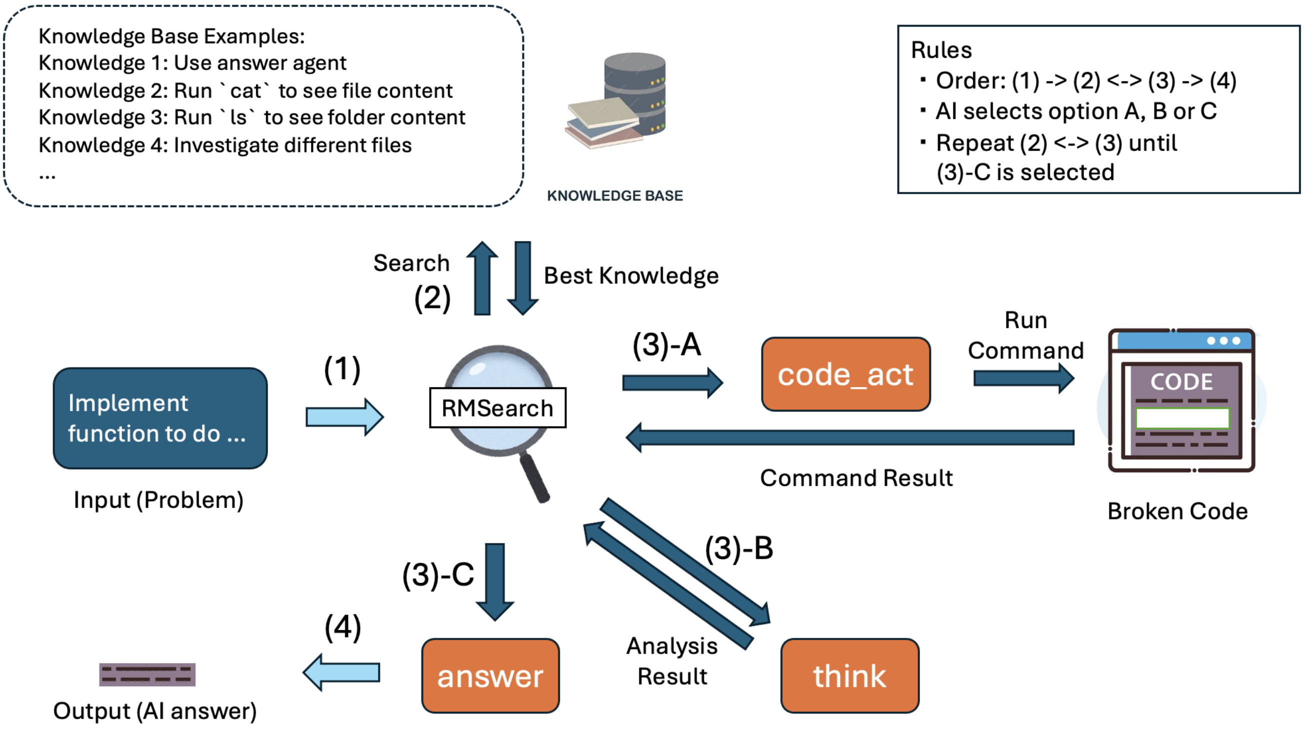

Figure | SEIMEI approach to access code base and solve problem.

We implement the inference loop using SEIMEI. (GitHub)

There are basically 3 agents used in analyzing gkv code.

- **code_act agent**: runs unix command (ex. `cat`, `ls`, `rg`) or python code to analyze local folder and files.
- **think agent**: see all command results and analysis results before, provide thought and decide what to do next.
- **answer agent**: gives final answer summarizing all the analysis result of code_act agent

This aligns with patterns demonstrated in prior agent work for tool use and repository-scale editing:

- **ReAct**-style reasoning+acting loops for stepwise progress. (GitHub)
- Tool-augmented LMs (Toolformer) and modular systems (MRKL). (arXiv)
- SWE-agent shows that carefully designed “agent–computer interfaces” improve code-editing success on benchmarks. (arXiv)
- OpenHands is an example of an open platform focused on coding agents. (GitHub)

Compared to the methods above, SEIMEI has an additional feature, **Routing and augmentation:** at each step, SEIMEI can call RMSearch to retrieve domain-relevant knowledge snippets, then incorporate them into the next model call. (GitHub)

We use RMSearch for integrating search model rather than conventional semantic-embedding model. It is because RMSearch, often refered to as reranker model, calculates relevance-score more directly and therefore is more adaptable to specific domain than semantic-embedding model. (GitHub)

3.4 Knowledge Generation

Knowledge pool is generated in two steps:

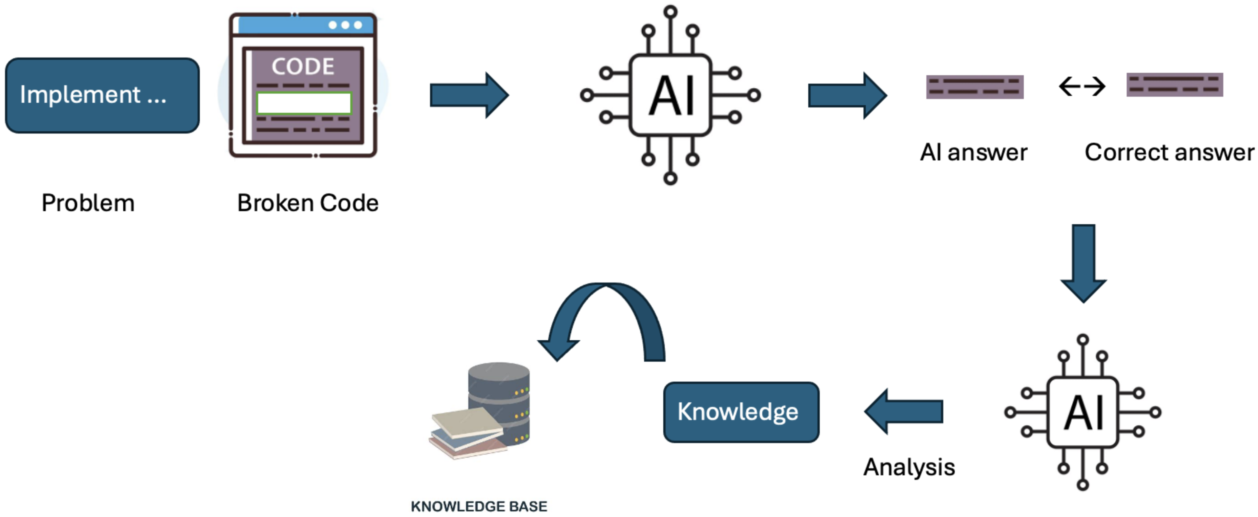

Figure | Knowledge update pipeline from correct answer.

1. **Manual knowledge:** Domain experts (or careful readers) write concise instructions about the task such as:

    - "Run answer agent because enough agent outputs are obtained."
    - "Run `ls` command to see what are in current folder."
    - "Run `cat` command to see what's inside a file."
    - "Run `rg` command to search keywords over a folder."
    - "Change the strategy to solve the question to file-comparison-centered analysis."

    Writing this requires careful analysis of reasoning steps and AI answers.

2. **Automatic knowledge update (from repairs):** Compare the agent's output patch to the expected fix and extract reusable statements such as:

    - "When you act on `cat` command, act `ls` first to check file path in the current folder."
    - "You often cause errors with `rg` command. Be sure to follow the format: __."
    - "When modifying the gyroaveraged potential term, also update normalization in ___."
    - "This file assumes flux-tube geometry; boundary conditions are enforced in ___."

    The goal is to turn "one solved instance" into a hint that helps future instances.

We keep both because automatic knowledge can scale, while manual knowledge can be higher precision.

3.5 Knowledge Sampling for RMSearch Dataset

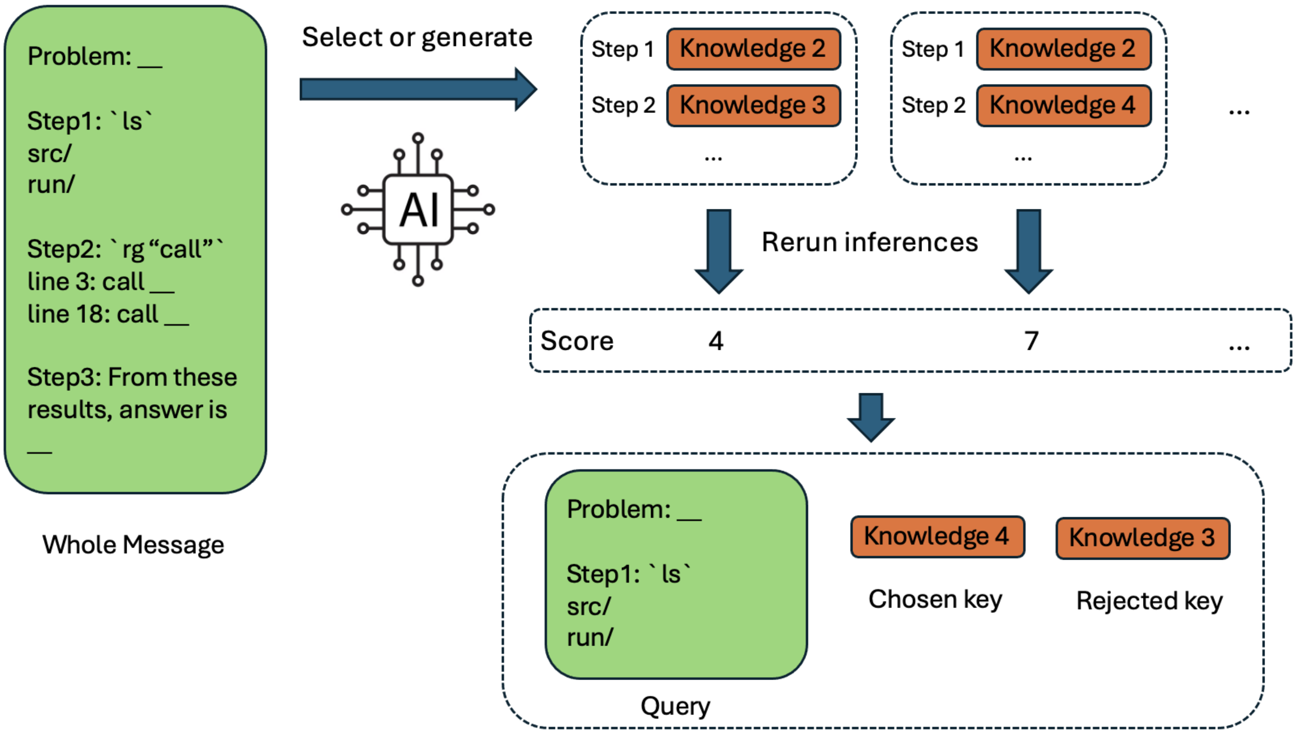

Figure | Preference-style dataset creation for DPO training (conceptual).

RMSearch training requires a preference-style dataset. We construct it from pipeline runs by creating comparisons like:

- **Knowledge preference:** given a query ("fix this missing physics term") and previous agent outputs, compare two candidate knowledge snippets A vs B based on whether using them leads to a higher-scoring answer.

This matches the general "learning from preferences" paradigm used in RLHF, but we apply it to **retrieval/reranking and agent routing** rather than directly to the generator model. (arXiv)

In this method, knowledge sampling and preference assignment are key. The sampling procedure used in this experiment is:

- **Knowledge generation or selection:** from the full message history of a base inference trial, an LLM generates or selects knowledge for designated steps. A set of knowledge texts spanning several steps is called a **knowledge chunk**. We generate multiple chunks for each problem.
- **Rerun inferences with knowledge chunks:** using each generated or selected knowledge chunk, rerun the inference. Several runs are performed per chunk.
- **Scoring knowledge chunks:** score each inference run and average scores per knowledge chunk to obtain a chunk-level score.
- **Converting to a preference dataset:** from chunk scores, build (query, chosen knowledge, rejected knowledge) pairs. The query is the message history up to the step that will be augmented by the chosen or rejected knowledge. A threshold removes trivial score differences.

3.6 RMSearch Training

3.6.1 Reward Design

The biggest feature of SEIMEI pipeline is that RMSearch is trained on reward given to inference answer. This makes SEIMEI pipeline different from basic RAG approach.

The reward is generated by comparing AI answer with original patch. Here's the reward (max 10) construction:

- +2: for modifying the correct file.
- +2: for modifying the same part as the correct one.
- +3: for writing the same functional code as a deleted part.
- +3: for how directly knowledge texts contribute to the reasoning steps. (+1 if knowledge identifies the correct file, +1 if knowledge identifies the correct code snippet, +1 if knowledge contributes the entire reasoning improvement).

3.6.2 Loss Function

RMSearch is trained with **DPO-style preference optimization**, treating the RMSearch as a model that should assign higher relevance-score to preferred items (knowledge snippets or patches). (arXiv)

Concretely, RMSearch implements a scoring function that maps a **query + key** pair to a scalar reward/score, i.e., $s_{\theta}(q, k) \rightarrow r$. For a preference triple (q, k^+, k^-), we use the DPO loss:

$$ \mathcal{L}_{\mathrm{DPO}} = -\log \sigma\left(\beta\left[s_{\theta}(q,k^+) - s_{\theta}(q,k^-)\right]\right) $$

where q is the query, k^+ is the preferred key (knowledge or candidate patch), k^- is the less-preferred key, s_{θ} is the RMSearch score (reward) function, s_{ref} is a fixed reference scorer used to keep updates conservative, β controls the sharpness of the preference margin, and σ is the logistic function. This makes the connection to RMSearch explicit: training adjusts the **query + key -> reward** scores so that preferred knowledge/patches receive higher scores, which directly improves the reranking behavior at inference time.

3.6.3 Batch construction (following InstructGPT's reward model training recipe).

A practical issue in preference training is that many pairwise comparisons derived from the *same* query are highly correlated. In the InstructGPT reward-modeling pipeline, labelers rank ${K}$ candidate completions per prompt (with ${K}$ between 4 and 9), yielding up to $\binom{K}{2}$ pairwise comparisons; the authors found that naively shuffling these comparisons and training on them as independent datapoints caused rapid overfitting. Instead, they treat **all $\binom{K}{2}$ comparisons from a single prompt as one batch element**, which is both (i) **more compute-efficient** (one forward pass per candidate rather than $\binom{K}{2}$ passes) and (ii) **more stable** (reduced overfitting, improved validation loss/accuracy). We adopt the same batching principle for RMSearch: each minibatch contains (B) distinct queries, and for each query we score ${K}$ candidate keys and apply the pairwise preference loss over the within-query comparison set, rather than mixing comparisons across queries indiscriminately. This keeps updates aligned with the "within-query reranking" structure that RMSearch must solve at inference time. (arXiv)

3.7 Training Iteration

- RMSearch is trained on SEIMEI inference and SEIMEI inference is on RMSearch model. This fact enables a training loop between inference improvement and RMSearch training.
- Here's the logic:
    1. RMSearch is trained on seimei inference sampling.
    2. Trained RMSearch improves knowledge retrieval and dataset sampling, which makes better dataset.
    3. This improved dataset trains more accurate RMSearch.

3.8 RMSearch & SEIMEI Evaluation

Important metrics on RMSearch evaluation

- Evaluation Loss: loss defined in 3.6.2, which is a target fiunction to be decreased.
- Accuracy: accuracy of predicting the correct key from given query.

SEIMEI inference pipeline is evaluated by score constructed in the same way as the reward (3.6.1).

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4. Experiment

We evaluate our models on dataset generated by the method in section 3.2. with a single plasma-simulation-library, GKV. 25

Dataset size:

- All Problems: 113
- Train Problems: 85
- Test Problems: 28

Models:

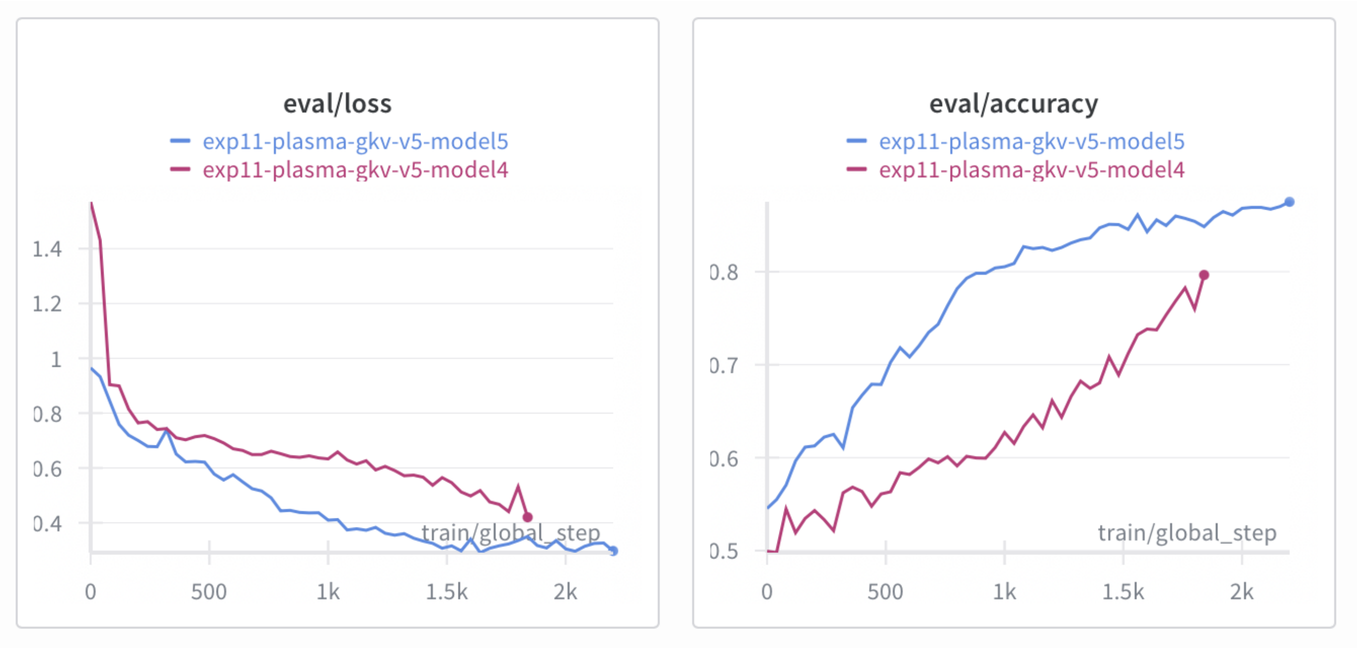
- Inference model: "openai/gpt-oss-20b"
- Reward model: "Skywork/Skywork-Reward-V2-Qwen3-4B" (will be called "qwen4b-reward")

Hyper parameters used in this experiment:

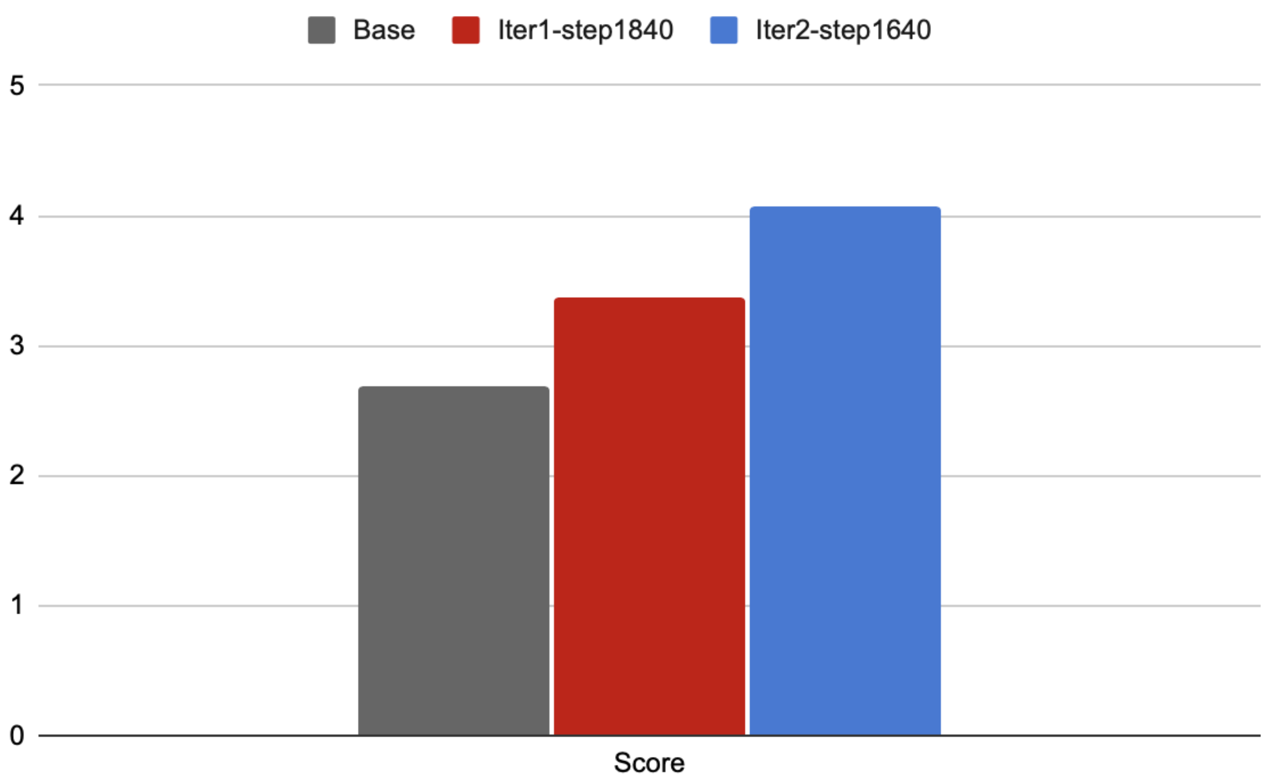
- Evaluation
    - Sampling numbers: 7
- Training
    - Score preference threshold: 0.5
- Iteration 1
    - Knowledge sampling model: "gpt-oss-20b"
    - Distribution decay rate: 0.8
    - Random knowledge sampling rate: 0.1
    - Sampling numbers: 14

- Iteration 2, 3
    - Knowledge sampling model: RMSearch trained in the previous iteration.
    - Distribution decay rate: 0.5
    - Random knowledge sampling rate: 0.1
    - Sampling numbers: 14

4.1. RMSearch Evaluation



4.2. SEIMEI Evaluation



4.3. Human Evaluation

4.4. GPU and Cost

- gpt-oss-20b: RTX A5000 24GB VRAM
- qwen4b-reward (Search): RTX A5000 24GB VRAM
- qwen4b-reward (Training): A40 48GB VRAM

For each iteration,

- 6h: knowledge sampling (2 RTX A5000 GPUs)
- 6h: training (1 A40 GPU)

which ended up with consuming roughly $6 per iteration. (Runpod Rental Server)

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5. Discussion

5.1. Interpretation of Experimental Reaults

- This is quite promissing result because this means that if a developper inputs a single library into SEIMEI and it automatically improves the whole system by more than 10%.

- As a current paradigm of reinforcement learning, it only improves the output LLM originally has. But in this method, RMSearch integrates knowledge as well and introduce a new output LLM didn't have.

- The fact that the accuracy improved over iteration loop shows that this system can improve itself constantly by acting and learning without getting overlearning.

- The learning cost is extremely cheaper than training on next token generation task. This is because searching knowledge is much more direct to adapt to a task than training next token generation.

5.2. Unsuccessful Attempts

When generating dataset and sampling knowledge, we also encountered failures and setbacks along the way. We share our failure experiences here to provide insights, but this does not imply that these approaches are incapable of developing effective search models.

5.2.1 Monte Carlo Tree Search (MCTS)

In the early stages of knowledge sampling method, we integrated MCTS by constructing step by step knowledge scoring, but this didn't go well, since the reward accuracy was quite bad and the system couldn't evolve meaningfully.

5.2.2 Knowledge Chunks Reward

To overcome the step by step rewarding failure, we introduced a concept "knowledge chunk". Knowledge chunk is a collecton of knowledge for different steps and generated by LLM analyzing base inference. In this method, score is defined for knowledge chunk, instead of a knowledge text in every step, and this leads to more solid reward. Even though this method shows some constant improvement, knowledge is made despite of LLM inference in each step, which often supresses flexible knowledge sampling.

5.2.3 Make dataset with codex

5.3. Possibility of Domain Specific LLM

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6. Conclusion

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