

000 001 002 003 004 005 STARK: STRATEGIC TEAM OF AGENTS FOR REFINING 006 KERNELS 007 008 009

010 **Anonymous authors**
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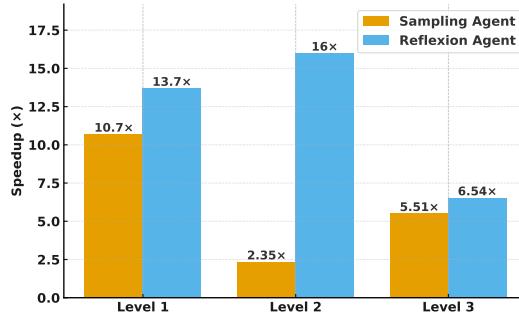
027 ABSTRACT

028 The efficiency of GPU kernels is central to the progress of modern AI, yet optimizing
029 them remains a difficult and labor-intensive task due to complex interactions
030 between memory hierarchies, thread scheduling, and hardware-specific character-
031 istics. While recent advances in large language models (LLMs) provide new op-
032 portunities for automated code generation, existing approaches largely treat LLMs
033 as single-shot generators or naive refinement tools, limiting their effectiveness in
034 navigating the irregular kernel optimization landscape. We introduce an LLM
035 agentic framework for GPU kernel optimization that systematically explores the
036 design space through multi-agent collaboration, grounded instruction, dynamic
037 context management, and strategic search. This framework mimics the workflow
038 of expert engineers, enabling LLMs to reason about hardware trade-offs, incor-
039 porate profiling feedback, and refine kernels iteratively. We evaluate our approach
040 on KernelBench, a benchmark for LLM-based kernel optimization, and demon-
041 strate substantial improvements over baseline agents: our system produces correct
042 solutions where baselines often fail, and achieves kernels with up to 16 \times faster
043 runtime performance. These results highlight the potential of agentic LLM frame-
044 works to advance fully automated, scalable GPU kernel optimization.

045 1 INTRODUCTION

046 Artificial intelligence (AI) has advanced at
047 an unprecedented pace, transforming both re-
048 search and real-world applications. While in-
049 novations in model architectures and training
050 algorithms have been central to this progress,
051 the efficiency of the computational infrastruc-
052 ture that executes them is equally critical. At
053 the core of modern AI systems are *GPU kernels*,
054 which implement fundamental operations
055 such as matrix multiplication and convolution.
056 Even modest improvements in GPU kernel effi-
057 ciency can translate into significant reductions
058 in training time, inference latency, and deploy-
059 ment cost, making kernel optimization a corner-
060 stone for sustaining AI’s rapid growth.

061 Despite their importance, designing and opti-
062 mizing GPU kernels remains a major challenge.
063 The performance of a kernel depends on sub-
064 tle interactions between thread scheduling, memory
065 hierarchy utilization, synchronization, and
066 hardware-specific characteristics. Small changes in tiling
067 strategies, loop unrolling, or memory
068 alignment can yield disproportionate effects on runtime. As a result, the kernel optimiza-
069 tion landscape is highly irregular, architecture-dependent, and difficult to navigate. Existing approaches
070 largely fall into two categories: *manual optimization* by expert engineers, which is effective but
071 labor-intensive and difficult to scale; and *automated compilers and domain-specific languages*
072 (DSLs) such as TVM and Triton (Chen et al., 2018; Tillet et al., 2019), which apply heuristics or
073 search but often struggle with irregular operators and hardware variability (Zheng et al., 2020a;b).



074 **Figure 1: Speedup of STARK over baseline agents**
075 **on KernelBench (L1-L3) with same number of at-
076 tempts.** Bars report GPU wall-clock speedups (x) re-
077 lative to the *Sampling* and *Reflexion* agents; higher is
078 better. STARK reaches up to 16 \times over Reflexion (L2)
079 and 10.7 \times over Sampling (L1).

The rapid progress of large language models (LLMs) opens a new opportunity for kernel optimization. Beyond their ability to generate correct code, LLMs can be guided to reason about hardware trade-offs, adapt to profiling feedback, and iteratively refine implementations. However, prior work has mostly treated LLMs as single-shot code generators or simple refinement tools (Ouyang et al., 2025), which underutilizes their potential for structured exploration of the kernel design space. To build a more powerful agent, we identify and address three critical limitations in existing methods:

1. **Naive exploration strategy.** Current agents typically refine code linearly, learning only from the immediately preceding attempt. This simplistic process neglects the rich history of prior attempts and fails to effectively balance the exploration-exploitation trade-off, often getting trapped in local optima.
2. **Monolithic agent design.** Kernel optimization is a multifaceted task requiring distinct capabilities for planning, implementation, and reflection. By assigning all these responsibilities to a single, generalist LLM, current agents operate inefficiently.
3. **Planning-implementation gap.** We observe a failure mode particularly acute in this domain: LLMs frequently devise a correct high-level optimization plan (e.g., “apply memory tiling”) but fail to translate it into valid low-level CUDA code. This gap stems from the relative scarcity of expert-level kernel code in the models’ training data.

To address these limitations, we introduce **STARK** (*Strategic Team of Agents for Refining Kernels*), a novel framework for automated GPU-kernel optimization. Our contributions are threefold:

- **Collaborative multi-agent workflow.** We design a workflow with specialized agents for planning, coding, and reflection, mirroring an expert development cycle and overcoming the inefficiencies of monolithic designs.
- **Bridging the planning-implementation gap.** We propose two mechanisms—*grounded instruction* and *dynamic context windows*—that translate high-level strategies into precise, actionable code edits, ensuring robust coordination across agents.
- **Strategic search for refinement.** We incorporate a search policy that balances exploration and exploitation over prior attempts, enabling systematic discovery of strong kernels.

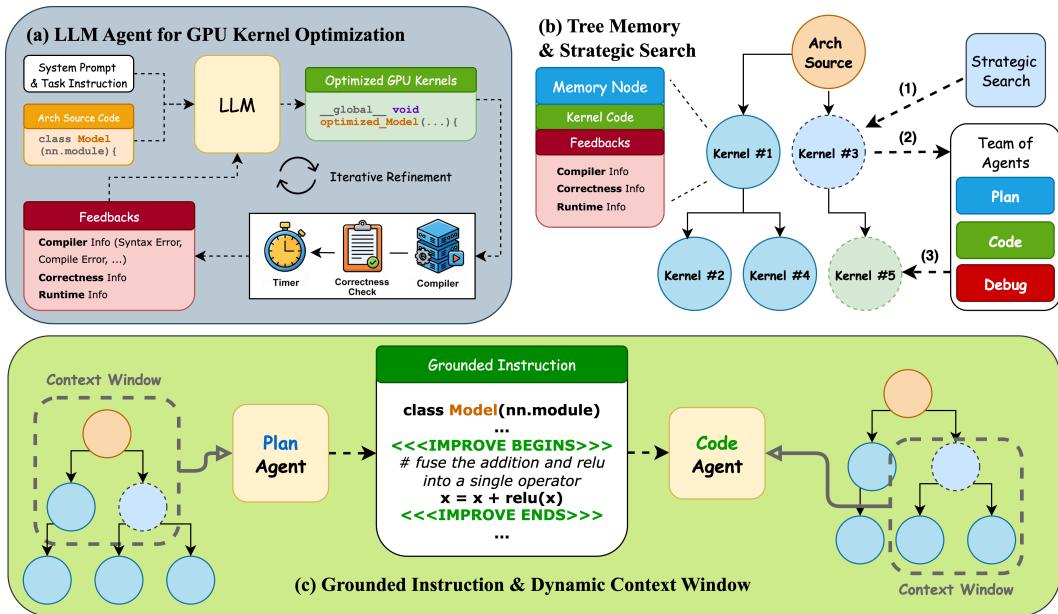


Figure 2: Overview of STARK. (a) Prior LLM-based kernel optimizers rely on a monolithic agent with local iterative refinement. (b) STARK replaces this with a collaborative multi-agent workflow (plan/code/debug) coupled with strategic search over a tree memory. (c) The plan agent issues *grounded instructions* that anchor edits to code spans; *dynamic context windows* surface role-specific history; and the debug agent repairs failures. See Section 4 for details.

We evaluate our framework on **KernelBench** Ouyang et al. (2025), a benchmark designed to assess LLM-based GPU kernel optimization. Experiments show that combining these improvements leads to an agent system significantly more competitive than the baseline agents in both runtime performance and success rate across diverse kernel problems, authoring competitive kernels for the challenging problems in KernelBench where the baseline agents struggle to even find a working solution. Notably, STARK achieves more than $10\times$ speedup over kernels produced by the baseline agents (i.e., the optimized kernels run in under one-tenth the time of the baseline.). Overall, our work suggests that LLM-driven agents represent a promising step toward fully automated GPU kernel optimization.

2 RELATED WORK

Due to space constrain, we only review the most relevant prior work here and defer the complete discussion to Appendix E.

The optimization of GPU kernels has progressed from empirical auto-tuning frameworks that perform black-box parameter searches (van Werkhoven, 2019; Nugteren & Codreanu, 2015) and compiler-based approaches with static heuristics (Yang et al., 2010), to the use of machine learning (ML). ML-based techniques have been used to replace hand-tuned heuristics in production compilers (Trofin et al., 2021), learn cost models to guide optimization (Chen et al., 2018), and even learn directly from raw source code without manual feature engineering (Cummins et al., 2017). A significant leap was the use of deep reinforcement learning to discover fundamentally new algorithms, as demonstrated by AlphaTensor’s success in finding faster matrix multiplication methods (Fawzi et al., 2022). While powerful, these prior works either optimize within a fixed search space or operate in purely formal domains. Our work addresses these limitations by operating directly on source code to implement novel, structural changes.

The emergence of powerful Large Language Models (LLMs) has revolutionized programmatic interaction with source code, demonstrating a remarkable proficiency in generating code for diverse applications from competitive programming to compiler testing (Gu, 2023; Zhong & Wang, 2024; Jain et al., 2025). This capability has catalyzed a paradigm shift away from single-shot code generation and toward the development of autonomous LLM agents. An agent enhances a base LLM with planning, memory, and tool-use capabilities to direct its own workflow (Weng, 2023). The success of frameworks like SWE-agent in independently resolving complex GitHub issues has validated the power of this approach for software engineering (SWE) (Yang et al., 2024). While the application of LLM agents to SWE is a burgeoning field of research (Yang et al., 2024; Antoniades et al., 2024; Yang et al., 2025), their potential in the specialized domain of GPU kernel optimization remains largely unexplored. To fill this gap, we designed STARK, an agent framework with capabilities tailored to the unique challenges of this domain.

3 PRELIMINARY

3.1 LLMs AND AUTOREGRESSIVE GENERATION

Given an input sequence $x = (x_1, x_2, \dots, x_n)$ (e.g., the task instruction) as the context, an LLM p_θ with parameters θ generates an output sequence $y = (y_1, y_2, \dots, y_m)$ where $y_t \in \mathcal{Y}$, $t \in \{1, \dots, m\}$ are tokens. Pretrained on a massive corpus of text, LLMs autoregressively generate the next token y_t conditioning on x and all the previously generated token $y_{<t} = (y_1, \dots, y_{t-1})$. Specifically, at each time t , the LLM first computes the logits $z_\theta(y|y_{<t}, x)$ for each token y in the vocabulary \mathcal{Y} and generate y_t following the conditional distribution

$$p_\theta(y_t|y_{<t}, x) = \frac{\exp(z_\theta(y_t|y_{<t}, x)/\tau)}{\sum_{y' \in \mathcal{Y}} \exp(z_\theta(y'|y_{<t}, x)/\tau)}. \quad (1)$$

The temperature parameter $\tau > 0$ modulates the randomness of an LLM’s output. Higher values of τ flatten the next token distribution in Equation 1, encouraging creative and diverse responses. Conversely, lower values sharpen the distribution, promoting deterministic and high-fidelity outputs.

This trade-off is critical in complex tasks, as different sub-problems demand different behaviors. For instance, **planning** and **exploration** benefit from a high temperature to generate novel strategies,

162 whereas tasks requiring precision and factual correctness, such as **code implementation**, necessitate
 163 a low temperature to ensure reliability. A single agent with a fixed temperature is ill-equipped to
 164 handle this dichotomy. This observation is a core motivation for STARK’s multi-agent design, which
 165 allows specialized agents to operate at distinct temperatures tailored to their roles, i.e., a high τ for
 166 the creative plan agent and a low τ for the precise code agent.

167
 168 **3.2 KERNELBENCH**
 169

170 **KernelBench** Ouyang et al. (2025) is a recently proposed benchmark specifically designed for as-
 171 sessing LLM-based GPU kernel optimization. Unlike prior evaluations that focus only on code cor-
 172 rectness or small-scale operator tests, KernelBench provides a principled and reproducible testbed
 173 that measures both correctness and runtime efficiency across a broad spectrum of GPU workloads.
 174 KernelBench comprises a suite of optimization tasks, categorized into three difficulty levels. For
 175 each task, the objective is to create a custom GPU kernel that is functionally equivalent to a pro-
 176 vided PyTorch reference implementation while minimizing its wall-clock execution time. See an
 177 example of the KernelBench task in Appendix D.

178 Specifically, **Level 1** tasks focus on single, common operators such as matrix multiplication and
 179 convolution, serving as a baseline for fundamental optimization capabilities; **Level 2** tasks com-
 180 prise tasks with multiple operators fused into a single kernel, testing the ability to manage more
 181 complex dataflows and scheduling; **Level 3** tasks represent the highest difficulty, featuring popular
 182 full ML architectures such as the ResNet (He et al., 2016) and LSTM (Hochreiter & Schmidhuber,
 183 1997), which involve highly irregular computations and intricate memory access patterns that are
 184 challenging for both human experts and automated systems to optimize effectively.

185
 186 **4 STARK: STRATEGIC TEAM OF AGENTS FOR REFINING KERNELS**
 187

188 **Framework Overview.** We now present STARK, an agentic framework for GPU-kernel optimiza-
 189 tion. STARK organizes kernel refinement into three layers: (i) a *multi-agent workflow* that separates
 190 planning, coding, and debugging, (ii) *coordination mechanisms* with *grounded instruction* to anchor
 191 planned edits to concrete code spans and *dynamic context windows* that surface role-specific history
 192 (e.g., prior attempts, failures, profiler feedback) to each agent, and (iii) a *strategic search* policy that
 193 balances exploration and exploitation across iterative attempts. Notably, multi-agent workflow and
 194 grounded instruction improve reliability even under a single-attempt budget, whereas dynamic con-
 195 text windows and strategic search deliver most of their gains when multiple attempts are allowed.
 196 Figure 2 provides an overview; the following subsections detail each component in turn.

197
 198 **4.1 MULTI-AGENT COLLABORATION**

199 Optimizing GPU kernels is inherently multifaceted and mirrors expert team workflows. A single
 200 agent typically fails to balance correctness, performance, and exploration across a vast, irregular
 201 design space. In particular, *strategy discovery* (e.g., fusion, vectorization, shared-memory tiling)
 202 benefits from higher-temperature generation that encourages diversity whereas *strategy realization*,
 203 i.e., committing those ideas to code, requires low-temperature precision to avoid errors. We therefore
 204 adopt a multi-agent framework that enables role specialization through LLMs.

205 **Multi-Agent Design (MAD).** Specifically, STARK decomposes kernel optimization into three roles
 206 – *plan*, *code*, and *debug*. Using a role-specific context window (Section 4.4) with selected prior
 207 attempts and execution outcomes, the **plan** agent proposes targeted transformations to either the source
 208 kernel or a candidate chosen by the strategic search policy (Section 4.2), emitting *grounded instruc-
 209 tions* (Section 4.3) that anchor edits to explicit code spans. The **code** agent consumes grounded
 210 instructions and translates them into executable GPU-kernel code, conditioning on its own context
 211 window to improve adherence and code quality. The **debug** agent repairs promising but failing can-
 212 didates by consulting the plan agent’s instructions and compiler/runtime diagnostics, producing a
 213 working kernel that realizes the intended transformation.

214 **Benefits of MAD.** Role specialization lets each agent use prompts and base LLMs matched to its ob-
 215 jective. In our instantiation, we choose Claude Sonnet 4 with temperature $\tau=0.8$ for the plan
 agent to encourage strategy diversity, and the same model with $\tau=0.1$ for the code and debug agents

216 to enforce precision. Despite this simple setup, MAD already performs strongly (see Section 5).
 217 We underscore that because the design is modular, we can swap in planners with richer kernel-
 218 optimization priors or code-specialist reasoning models to further improve results. In addition,
 219 modularity also exposes bottlenecks. We observe that the dominant bottleneck is code-synthesis
 220 fidelity: LLMs often need multiple attempts to faithfully implement a given instruction. Finally,
 221 MAD makes targeted post-training straightforward: we can fine-tune the base LLM for a specific
 222 agent (e.g., the code agent) *without* affecting the others, improving stability and predictability. How-
 223 ever, a systematic study of agent-specific post-training is orthogonal to our core contributions and
 224 is left to future work.

225 226 4.2 STRATEGIC SEARCH WITH TREE MEMORY

227 Prior LLM-driven kernel optimizers typically use either *best-of- K* sampling that generates multiple
 228 candidates independently and select the fastest correct one or *iterative refinement* which repeatedly
 229 edits the latest kernel (Ouyang et al., 2025). However, best-of- K is unguided and wasteful: all the
 230 new attempts ignore feedback from earlier attempts and repeatedly probe redundant regions of the
 231 design space. On the other hand, iterative refinement is feedback-aware but *myopic*: by building
 232 only on the most recent candidate, it is prone to getting trapped in narrow, suboptimal basins.

233 To address these limitations, STARK reframes kernel optimization as **strategic search** over a persistent
 234 **tree memory**. We maintain a search tree T whose nodes store candidates and their observations
 235 (runtime, correctness, and compiler diagnostics). The root represents the source architecture; each
 236 edge corresponds to applying a grounded instruction from the plan agent and realizing it via the code
 237 agent (or repairing via the debug agent). Each node n is assigned a score $s(n)$ reflecting competi-
 238 tiveness; in our implementation we use the straightforward kernel runtime as $s(n)$ and treat *lower*
 239 is *better*. For kernels that are incorrect or failing to compile, we give them scores of $+\infty$. At each
 240 step, we (1) *select* a node to expand using a strategic policy, (2) *expand* by invoking the plan/code (or
 241 debug) agents to produce a child candidate, (3) *evaluate* for correctness and runtime, and (4) *record*
 242 results in T to inform subsequent selections. This converts ad-hoc trial-and-error into a directed,
 243 feedback-driven process.

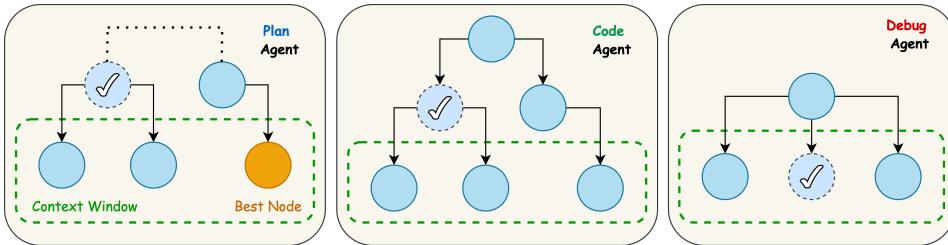
244 **Policy choice and an adapted ϵ -greedy rule.** We compared representative search policies includ-
 245 ing Monte-Carlo Tree-Search (MCTS), evolutionary, greedy, and ϵ -greedy policies and found that
 246 ϵ -greedy consistently performs best under the same budget constraint. Importantly, we observe that
 247 kernel optimization poses domain-specific challenges that are root dominance (it is very challeng-
 248 ing to even outperform the source architecture in the root node) and frequent compilation/runtime
 249 failures. To address these challenges, we adapt the canonical rule as follows: (1) **Root throttling**:
 250 cap the number of direct children of the root at n_{root} to avoid redundant first-hop edits; once the cap
 251 is reached, the root is ineligible for selection; (2) **Dead-branch pruning**: if a node has more than
 252 n_{child} children and all current children fail, mark the node ineligible to prevent wasting trials; (3)
 253 **High exploration rate**: use a relatively large ϵ (empirically 0.3–0.4) to counteract local traps; (4)
 254 **Leaf-biased exploration**: with probability ϵ , sample uniformly from expandable leaves (not only
 255 failing nodes), encouraging discovery beyond the immediate failure set.

256 257 258 4.3 GROUNDED INSTRUCTION

259 We introduce grounded instruction for kernel enhancement. The plan agent must not only pro-
 260 pose an optimization, but also insert **explicit span anchors** in the kernel source that mark
 261 exactly where the change should occur. Each anchor is a short, machine-checkable tag (i.e.,
 262 <<<IMPROVE BEGINS>>> ... <<<IMPROVE ENDS>>>) wrapped around the target site, such
 263 as a load/store, loop body, or the launch configuration. The code agent consumes this annotated scaf-
 264 fold and resolves each anchor by emitting concrete CUDA that realizes the instruction. Grounded in-
 265 struction tightens plan–code alignment, curbs hallucinated guidance, and narrows the coder’s search
 266 space. It also improves traceability: every proposal leaves a visible, verifiable footprint in the final
 267 code. In practice, we observe fewer misinterpretations and markedly fewer faulty kernels. Despite
 268 its simplicity, the mechanism is especially effective on Level 3 KernelBench tasks with deeper ar-
 269 chitectures (e.g., VGG).

270 4.4 DYNAMIC CONTEXT WINDOW
271

272 Past attempts provide rich, actionable signals for subsequent decisions, but different agents ben-
273 efit from different *views* of this history. We therefore maintain a *dynamic, agent-specific context*
274 *window* that is rebuilt at each selection step for different agents. See Figure 3 for a visual demon-
275 stration. Throughout this section, let node i be the node selected by the search policy defined in
276 Section 4.2. We use $\mathcal{W}(i)$ to denote the context window containing a subset of historical attempts
277 and their evaluation outcomes (e.g., compiler information and runtime). As we always include the
278 source architecture as part of the prompt for agents, $\mathcal{W}(i)$ always includes the root node n_{root} . For a
279 naive search algorithm without dynamic context window, $\mathcal{W}(i) = \{i, n_{\text{root}}\}$ only includes node i in
280 addition to the root.

281 **Figure 3:** Dynamic Context Window. Nodes with √'s represent selected nodes.
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289 **Tree relations.** We use tree relations to build agent-specific context windows. Let $p(i)$ be the parent
290 of node i . Define the *siblings* of i as $\mathcal{S}(i) = \{j : p(j) = p(i)\}$. Moreover, define the set of child
291 nodes of a node i as $\mathcal{D}(i)$. We also maintain a small global leaderboard \mathcal{C} of top-performing nodes.
292

293 **Plan agent (local & contrastive global context).** For a selected node i , the plan agent conditions
294 on a context window $\mathcal{W}_{\text{plan}}(i)$ that aggregates node i 's children and a small set of global leaders
295 from the leaderboard \mathcal{C} . Formally,

$$296 \mathcal{W}_{\text{plan}}(i) = \{i, n_{\text{root}}\} \cup \mathcal{D}(i) \cup \text{Top-}r(\mathcal{C}),$$

297 where $\mathcal{D}(i)$ contains all evaluated children of i with their observations, and $\text{Top-}r(\mathcal{C})$ returns the
298 r highest-scoring distinct kernels from the global leaderboard (excluding i 's subtree) to discourage
299 duplication.

300 This design serves three purposes. (i) **reflection**: the plan agent can revise or stack its prior instruc-
301 tions rather than rediscovering them; (ii) **ambition calibration**: top competitors prevent redundant
302 exploration and provide transferable motifs such as warp-shuffle reductions, vectorized LD/ST, and
303 shared-memory tiling; (ii) **capability estimation**: by inspecting how past instructions were real-
304 ized or failed by the code agent, the next instruction is adapted to what the code agent can reliably
305 execute, *improving first-pass success and avoiding instructions beyond current ability*. To achieve
306 this, we explicitly require the plan agent to adapt its instruction to the code agent's demonstrated
307 capabilities observed in $\mathcal{D}(i)$.

308 **Code agent (extended context).** For kernel code emission at node i , the code agent conditions on

$$309 \mathcal{W}_{\text{code}}(i) = \{i, n_{\text{root}}\} \cup \mathcal{D}(i) \cup \{j : p(j) \in \mathcal{S}(i)\}.$$

310 The nodes in $\{j : p(j) \in \mathcal{S}(i)\}$ are essentially the children of node i 's siblings. Our insight is that
311 these nodes typically share near-identical scaffolds with node i from a common planning lineage,
312 so successful patches and micro-optimizations transfer with high probability; conversely, seeing
313 failures in closely related contexts helps the coder avoid repeating the same mistakes. Hence, this
314 extended window serves two aims: (i) **reduce implementation errors** by letting the coder imitate
315 successful patches from closely related scaffolds and avoid previously observed failure modes; (ii)
316 **surface stronger implementations** by transferring micro-optimizations (e.g., warp-shuffle motifs,
317 vectorized LD/ST, shared-memory tiling) that have already worked on cousin nodes.

317 **Debug agent (local context).** For fault repair, we construct the context window for the debug code
318 as

$$319 \mathcal{W}_{\text{debug}}(i) = \{i, n_{\text{root}}\} \cup \mathcal{S}(i),$$

324 We choose this design mainly for two reasons. Most fixes are structural and local, e.g., off-by-
 325 one guards, stride/indexing alignment, launch-parameter tweaks, or shared-memory sizing often
 326 transfer directly among siblings that share the same scaffold. Moreover, restricting the window to \mathcal{S}
 327 avoids distracting the debug agent with globally unrelated kernels, improving precision and reducing
 328 hallucinated edits.

329

330 4.5 FRAMEWORK OVERVIEW

331

332 Here we provide an overview of our framework STARK and describe its execution process. Algo-
 333 rithm 1 presents its pseudocode.

334 At a high level, STARK repeatedly (i) selects a promising node (a prior attempt) from a search
 335 tree, (ii) builds agent-specific context windows from local history and global leaders, (iii) asks the
 336 *planning agent* to propose a concrete optimization along with *grounded instruction* anchors inserted
 337 into a scaffold, (iv) asks the *code agent* to realize those anchors into an executable kernel, (v) if
 338 the selected node has a problematic kernel, we build the debugger’s dynamic context window and
 339 request a minimal fix. The new attempt is evaluated, appended as a child node, and the leaderboard
 340 \mathcal{C} is updated. We repeat this process until we reach a pre-specified max attempts B .

341

342 **Algorithm 1** STARK: Strategic Team of Agents for Refining Kernels

343 **Require:** Budget B (max attempts), selection policy π_{select} (adapted ε -greedy), leaderboard size r

344 1: Initialize search tree T with root n_{root} (PyTorch reference)
 345 2: Initialize leaderboard $\mathcal{C} \leftarrow \{n_{\text{root}}\}$
 346 3: **for** $t = 1, 2, \dots, B$ **do** ▷ pick a node to refine
 347 4: $i \leftarrow \pi_{\text{select}}(T, \mathcal{C})$ ▷ compile fail or unit-test fail recorded at i
 348 5: **if** HASBUG(i) **then** ▷ compile fail or unit-test fail recorded at i
 349 6: $\mathcal{W}_{\text{debug}}(i) \leftarrow \text{BUILDCONTEXTDEBUG}(i, T)$
 350 7: $\text{kernel}' \leftarrow \text{DEBUGAGENT}(\mathcal{W}_{\text{dbg}}, i.\text{kernel}, i.\text{logs})$
 351 8: (ok , correct , runtime , logs) $\leftarrow \text{EVALUATE}(\text{kernel}')$ ▷ compile, correctness check,
 352 **timing**
 353 9: (plan , anchors) $\leftarrow (i.\text{plans}, i.\text{anchors})$
 354 10: **else**
 355 11: $\mathcal{W}_{\text{plan}}(i) \leftarrow \text{BUILDCONTEXTPLAN}(i, T, \mathcal{C})$
 356 12: (plan , anchors) $\leftarrow \text{PLANAGENT}(\mathcal{W}_{\text{plan}})$
 357 13: $\mathcal{W}_{\text{code}}(i) \leftarrow \text{BUILDCONTEXTCODE}(i, T)$
 358 14: $\text{kernel}' \leftarrow \text{CODEAGENT}(\mathcal{W}_{\text{code}}, \text{plan}, \text{anchors})$
 359 15: (ok , correct , runtime , logs) $\leftarrow \text{EVALUATE}(\text{kernel}')$
 360 16: **end if** ▷ fastest correct, grounded kernel
 361 17: $j \leftarrow \text{ADDCHILD}(T, i, \text{kernel}', \text{plan}, \text{anchors}, \text{ok}, \text{correct}, \text{runtime}, \text{logs})$
 362 18: $\mathcal{C} \leftarrow \text{UPDATELEADERS}(\mathcal{C}, j, r)$
 363 19: **end for**
 364 20: **return** $\text{BEST}(\mathcal{C})$ ▷ fastest correct, grounded kernel

365

366 5 EXPERIMENTS

367

368 We use KernelBench (Ouyang et al., 2025), a recently proposed benchmark consisting of compre-
 369 hensive and challenging GPU kernel tasks, to validate the effectiveness of our proposed approaches.

370

371 **Baselines and Metrics.** We compare our framework STARK with the following list of approaches:

372

- 373 • **Torch Eager:** the out-of-box PyTorch modules without any compilation or optimization.
- 374 • **Torch Compile :** We use `torch.compile` to produce optimized versions of the given
 375 PyTorch modules. While `torch.compile` offers different compilation modes, we compare to two of the most representative and competitive ones – **default** and **max-autotune**.
- 376 • **Sampling Agent:** the single agent framework originally proposed and used by Kernel-
 377 Bench to evaluate the difficulty of the tasks in KernelBench and the ability of LLMs to

378 write efficient kernels. This agent repeatedly samples responses when given the source
 379 model to optimize and chooses the best generated custom kernel as the solution.
 380

- 381 • **Reflexion Agent:** this agent follows the Reflexion paradigm (Shinn et al., 2023), where at
 382 each optimization step, it tries to update its last attempt using its corresponding observa-
 383 tions such as the compiler and runtime information.

384 We report the following metrics to comprehensively understand the agents’ performances: (i) **Fast₁**
 385 rate is the percentage of the problems for which the agent can generate kernels that are *at least* as
 386 fast as the torch baselines; (ii) **Success** rate represents the percentage of the problems for which the
 387 agent can generate compiled and correct kernels; (iii) **Speed**: To better understand how good the
 388 generated kernels are, we also report the average speed across all tasks.

389 **Comparison with Torch Baselines.** In Table 1, we present the results about success rate, **Fast₁**
 390 rate and speed over all 3 levels of KernelBench challenges. For each task, we let all agents to
 391 have a maximum of $B = 30$ attempts. Due to limited computation resource, we evaluate on the
 392 representative subset of KernelBench (Ouyang et al., 2025). We use Claude Sonnet 4 as the
 393 base LLMs for all the LLM-based baselines and our agents. Due to space constraint, we defer
 394 implementation and evaluation details to Appendix B.

395 The results in Table 1 demonstrate that our proposed framework, STARK, consistently outperforms
 396 both the Sampling and Reflexion baselines across all KernelBench difficulty levels. At Level 1,
 397 STARK not only achieves a perfect 100% success rate but also delivers up to a $3.0\times$ speedup over
 398 Torch Eager baselines, while Sampling and Reflexion agents frequently generate kernels that are
 399 slower than the baselines. This advantage becomes even more pronounced at Level 2, where the
 400 complexity of the kernels increases. Here, STARK maintains a perfect success rate and achieves
 401 speedups of $2.7\times$, whereas the Reflexion agent, despite attaining 100% correctness, produces ker-
 402 nels that run slower than the baseline. At Level 3, which involves the most irregular and challenging
 403 tasks, both Sampling and Reflexion degrade significantly, with success rates falling and runtimes
 404 dropping below baseline. In contrast, STARK continues to maintain full success while producing
 405 kernels that outperform the Torch implementations by up to $1.6\times$. These results highlight that
 406 STARK not only generates correct kernels but also delivers substantial performance improvements,
 407 even as task difficulty increases.

		Torch Eager		Default		Max-autotune	
Level 1	Success	Fast₁	Speed	Fast₁	Speed	Fast₁	Speed
Sampling Agent	57.1%	14.3%	0.81 \times	7.1%	0.46 \times	7.1%	0.81 \times
Reflexion Agent	92.6%	28.6%	1.24 \times	14.3%	0.57 \times	35.7%	0.92 \times
STARK	100%	71.4%	3.03 \times	78.6%	2.37 \times	78.6%	2.76 \times
Level 2	Success	Fast₁	Speed	Fast₁	Speed	Fast₁	Speed
Sampling Agent	87.5%	50%	1.06 \times	37.5%	0.91 \times	37.5%	0.91 \times
Reflexion Agent	100%	75%	0.88 \times	62.5%	0.78 \times	62.5%	0.78 \times
STARK	100%	100%	2.69 \times	87.5%	2.51 \times	87.5%	2.52 \times
Level 3	Success	Fast₁	Speed	Fast₁	Speed	Fast₁	Speed
Sampling Agent	100%	50%	0.87 \times	12.5%	0.67 \times	12.5%	0.66 \times
Reflexion Agent	67.5%	25%	0.79 \times	12.5%	0.62 \times	12.5%	0.61 \times
STARK	100%	87.5%	1.58 \times	87.5%	1.27 \times	87.5%	1.26 \times

424 **Table 1:** Performance of LLM Agents on the KernelBench Tasks. **Fast₁** represents the percentage of problems
 425 for which the agent can generate custom kernels that are correct and as fast as the Torch baselines (higher is
 426 better). Speed is computed as the ratio of the kernel runtime of the baseline to that of the generated kernel.

427
 428 **Comparison between Agents.** We investigate deeper into the behavior of our agent STARK with
 429 the two baseline agents to better understand their optimization behaviors. A deeper analysis of
 430 compile and correctness rates, shown in Table 2, provides further insight into why STARK succeeds
 431 where baselines struggle. While all agents achieve relatively high compile rates (mostly above 80%),

432 the fraction of kernels that are both compilable and correct varies widely. The Sampling agent,
 433 for example, compiles over 90% of its outputs on Level 1 but only 43% of these are functionally
 434 correct. Reflexion improves correctness slightly through iterative refinement, but its correctness
 435 rate remains below 55% at all levels. In contrast, STARK achieves the highest correctness rates
 436 across the board, reaching 61.2% on Level 2 tasks. This suggests that STARK’s structured planning
 437 and feedback-driven refinement not only increase the chance of generating efficient kernels but
 438 also reduce wasted attempts on invalid or incorrect code. Finally, Figure 1 highlights the dramatic
 439 runtime improvements of STARK relative to baseline agents. On Level 1 tasks, STARK achieves
 440 over a 10× speedup compared to Sampling and a 13.7× speedup over Reflexion. On Level 2, these
 441 gains rise as high as 16×, and even at the most challenging Level 3 tasks STARK maintains 5–6×
 442 improvements. These relative gains indicate that while baselines occasionally achieve correctness,
 443 they rarely deliver true runtime efficiency. By contrast, STARK’s ability to jointly optimize for
 444 correctness and speed allows it to close both gaps simultaneously. Taken together, these findings
 445 confirm that multi-agent collaboration and strategic search are key enablers for scaling LLMs to the
 446 demands of GPU kernel optimization.

KernelBench Level	Compile Rate↑			Correct Rate↑		
	1	2	3	1	2	3
Sampling Agent	90.8%	97.0%	84.9%	43%	44.0%	15.1%
Reflexion Agent	86.0%	86.2%	78.9%	48.3%	53.4%	28.4%
STARK	84.5%	90.7%	83.4%	50.6%	61.2%	35.5%

454 **Table 2:** Percentages of Successfully Compiled and Correct Kernels.
 455

456 **Ablations.** We ablate the agentic components of our system. We compare (i) **Search Agent**, which
 457 is a single-agent model equipped with our strategic search, and (ii) **MA-only**, which employs the
 458 multi-agent workflow (plan/code/debug with grounded instruction) using best-of- K sampling
 459 instead of search. As shown in Table 3, both variants outperform the *Sampling* baseline, confirming
 460 that each component helps. When combined in STARK, the effects compound: strategic search
 461 exploits the structured proposals produced by the multi-agent workflow, yielding the largest gains.
 462

	Torch Eager		Default		Max-autotune	
	Fast ₁ ↑	Speed↑	Fast ₁ ↑	Speed↑	Fast ₁ ↑	Speed↑
Sampling Agent	50%	0.87×	12.5%	0.67×	12.5%	0.66×
Search Agent	67.5%	0.89×	25%	0.71×	25%	0.70×
MA-Only	67.5%	1.11×	25%	0.92×	25%	0.91×
STARK	87.5%	1.58×	87.5%	1.27×	87.5%	1.26×

471 **Table 3:** Ablation on the Proposed Agentic Features.
 472

474 6 CONCLUSION

475 In this work, we introduced an agentic framework for GPU kernel optimization that combines multi-
 476 agent role play, dynamic context management, and strategic search. Our evaluation on KernelBench
 477 demonstrated that the proposed framework consistently outperforms baseline methods in both suc-
 478 cess rate and runtime efficiency, across tasks of varying complexity. These results highlight the
 479 value of moving beyond single-agent or unguided sampling approaches, and point to the promise
 480 of collaborative, feedback-driven optimization. Looking forward, we envision that agentic LLM
 481 frameworks will play an increasingly important role in automated system optimization. Extending
 482 our approach to broader classes of operators, diverse hardware architectures, and cross-kernel
 483 scheduling decisions are natural directions for future research. More broadly, our work suggests that
 484 multi-agent LLMs can meaningfully accelerate the co-design of AI algorithms and infrastructure,
 485 pushing the boundaries of what is possible in efficient large-scale computation.

486 ETHICS STATEMENT
487488 This study complies with the ICLR Code of Ethics. All datasets employed are publicly available
489 and open-source under licenses that permit research use. No private or personally identifiable in-
490 formation was accessed, and no new data were collected from human subjects. The research does
491 not pose privacy, security, or fairness concerns. The authors declare no conflicts of interest and no
492 external sponsorship.493
494 REPRODUCIBILITY STATEMENT
495496 We document all algorithmic and implementation details in the paper and appendix, including the
497 exact prompts for every agent, full hyperparameters, and ablation settings. Upon acceptance, we
498 will release an open-source repository with configuration files, an environment file and Dockerfile,
499 and step-by-step commands to recreate every table and figure.500
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648 **A USE OF LARGE LANGUAGE MODELS (LLMs)**
649650 Large Language Models (LLMs) were used solely as general-purpose assistive tools to improve the
651 clarity and readability of the manuscript. Specifically, we used an LLM to help rephrase and polish
652 text that we had already drafted.
653654 **B IMPLEMENTATION AND EVALUATION**
655656 **Agent Implementation.** We use Claude Sonnet 4 as the base LLMs for all agent baselines and
657 agents of STARK. For both sampling and reflexion agents, we follow KernelBench to set temperature
658 $\tau = 0.7$ during generating, with other generation parameters such as top-p set to the default value.
659 For STARK, we use Claude Sonnet 4 with temperature $\tau = 0.8$ for the plan agent, and $\tau = 0.1$
660 for the code and debug agents. For all tasks, all agent baselines and STARK have a maximum of
661 $B = 30$ attempts to optimize each task. Regarding the hyperparameters of STARK, we choose the
662 root throttling number to be 5, dead-branch pruning number to be 3, $\epsilon = 0.3$ for the search, $r = 2$
663 for the leaderboard \mathcal{C} . To prevent exploding context to the LLMs, we set an upper limit for the
664 number of nodes in the dynamic context window: whenever the dynamic context window has more
665 than 5 nodes, we randomly sample 5 from all the nodes in the window. We implement STARK with
666 LangGraph (LangChain Inc., 2025).
667668 **Runtime Evaluation.** We evaluate all the Pytorch baselines and LLM-generated kernels on the same
669 NVIDIA A100 40GB GPU. We use the source code provided by KernelBench at its official repo¹ to
670 benchmark the kernels’ runtime. In particular, to ensure stable measurement, runtime is measured
671 with CUDA events after warm-up runs using fixed input shapes; we choose a large number of 100
672 warm-up runs to ensure accurate measurement.
673674 **C PROMPTS**
675676 Our prompts follow the templates of KernelBench (Ouyang et al., 2025), which has four compo-
677 nents: *system message*, *in-context example*, *architecture source code*, and *instruction*.
678679 As we have multiple agents in STARK with different tasks, they require different prompts to fulfill
680 their tasks. Specifically, we reuse the system message and in-context example from KernelBench
681 for all agents and include the architecture source code regardless of which node is selected for opti-
682 mization. To motivate the agents to use the already optimized modules such as cuBLAS, we include
683 an additional instruction in the system message to consider using existing highly optimized kernels.
684 We show the system prompt in Figure 7, the in-context example in Figures 11 and 12. In addition,
685 we include the information within the *dynamic context window* and *role-specific instructions* for dif-
686 ferent agents. See Figure 4 for the prompt template of STARK. We show the role-specific instruction
687 in Figures 8, 9, and 10.
688689 **D EXAMPLE KERNELBENCH TASKS**
690691 Here we show three examples of KernelBench tasks, one for each level. See Figures 13, 14, and 15
692 for example tasks in Level 1, 2, and 3. We refer interested readers to Ouyang et al. (2025) for the
693 complete list.
694695 **E RELATED WORK**
696697 Optimizing GPU kernels to extract maximum performance from underlying hardware is a long-
698 standing and formidable challenge. The vast, non-convex, and hardware-specific search space of
699 possible kernel implementations necessitates sophisticated optimization strategies. The evolution of
700 these strategies can be broadly categorized into three paradigms: empirical auto-tuning, compiler-
701 and model-driven optimization, and most recently, generative approaches using Large Language
702¹<https://github.com/ScalingIntelligence/KernelBench>

```

702 1 {System Message}
703 2
704 3 Here's an example to show you the syntax of inline embedding
705 4 custom CUDA operators in torch: The example given architecture is:
706 5 {Example Architecture Source Code}
707 6 The example new arch with custom CUDA kernels looks like this:
708 7 {Example New Architecture Source Code}
709 8 You are given the following architecture:
710 9 {Architecture Source Code}
711 10
712 11 Here is your latest attempt:
713 12 {Source Code of the Selected Node}
714 13
715 14 [Dynamic Context Window] You should use the following observations
716 15 regarding your historical attempts to provide better
717 16 implementations:
718 17 - Learn from the failed examples to avoid bugs and write
719 18 successful kernels.
720 19 - Learn from the successful examples to design improved kernels.
721 20
722 21 **Kernel Source Code #1**
723 22 {Source Code of Historical Attempt}
724 23
725 24 **Compiler Observation**
726 25 {Compiler Log}
727 26
728 27 **Kernel Execution Result**
729 28 {Runtime or Correctness Error}
730 29
731 30 **Kernel Source Code #2**
732 31 [...skipped]
733 32
734 33 {Role-specific Instruction}

```

Figure 4: Prompt Template for Agents.

Models (LLMs). Our work builds upon this trajectory by introducing a fully autonomous agent that manages the entire optimization lifecycle.

E.1 EMPIRICAL AND COMPILER-BASED OPTIMIZATION

The foundational approach to GPU performance tuning is empirical auto-tuning, which treats the problem as a black-box search over a set of tunable parameters, such as thread block dimensions, memory tiling factors, and loop unrolling factors (van Werkhoven, 2019). Traditional methods often rely on an exhaustive or brute-force search, where thousands of potential kernel configurations are generated, compiled, and benchmarked to identify the top performer (Kurzak et al., 2012). While effective, this process is prohibitively time-consuming; for instance, an exhaustive search for a single GEMM kernel can take over 700 minutes to complete (NVIDIA Developer, 2024).

To mitigate this cost, heuristic-driven methods prune the search space. NVIDIA's `nvMatmulHeuristics`, for example, uses a predictive model to recommend a small subset of high-potential configurations, achieving near-optimal performance in a fraction of the time (NVIDIA Developer, 2024). Frameworks like Kernel Tuner (van Werkhoven, 2019), ATF (Rasch et al., 2017), and CLTune (Nugteren & Codreanu, 2015) provide robust environments for orchestrating these searches and support more advanced strategies like Bayesian Optimization, which builds a probabilistic performance model to guide the search more intelligently (Hellsten et al., 2023; Heldens & van Werkhoven, 2023).

Concurrently, compiler-based approaches aim to automate optimization through a series of program transformations applied to an intermediate representation (Yang et al., 2010). GPU compilers em-

```

756 1 ## System Message
757 2
758 3 You are an expert in writing efficient code.
759 4 You write custom CUDA kernels to replace the pytorch operators in
760 5 the given architecture to get speedups.
761 6 You have complete freedom to choose the set of operators you want
762 7 to replace. You may make the decision to replace some operators
763 8 with custom CUDA kernels and leave others unchanged. You may
764 9 replace multiple operators with custom implementations, consider
765 10 operator fusion opportunities (combining multiple operators into a
766 11 single kernel, for example, combining matmul+relu), or
767 12 algorithmic changes (such as online softmax). You are only limited
768 13 by your imagination.
769 14
770 15 You should consider using CUDA's existing highly optimized kernels
771 16 and operations whenever appropriate. Try building on these
772 17 optimized blocks and further improve it with your custom kernels.
773 18
774 19

```

Figure 5: System Message for All Agents.

```

775 1 ## System Message
776 2
777 3 You act as an LLM agent specializing in GPU optimization. Your
778 4 goal is to speed up a given PyTorch architecture by generating
779 5 custom CUDA kernels to replace its existing operators.
780 6 You may freely choose which operators to target, whether to
781 7 rewrite one operator, many operators, or none. You can pursue
782 8 kernel fusion opportunities (e.g., folding linear layers and
783 9 elementwise ops together) or restructure the computation
784 10 algorithmically to achieve higher throughput or lower memory
785 11 traffic.
786 12
787 13 There are no constraints on what transformations you may
788 14 propose innovation is encouraged.
789 15
790 16 Use CUDAs existing highly optimized kernel libraries whenever
791 17 advantageous; treat them as strong baselines that your custom
792 18 kernels can refine, fuse, or extend to achieve even greater
793 19 efficiency.
794 20
795 21

```

Figure 6: Alternate System Message V1 for STARK.

ploy passes for memory coalescing, data prefetching, vectorization, and loop optimizations to adapt naive code to the hardware architecture (Buck, 2008). While these approaches excel at finding optimal configurations within a predefined search space, they cannot fundamentally alter the kernel’s algorithm. Our work introduces an agent that reasons about performance bottlenecks to implement novel, structural code changes, moving beyond simple parameter tuning.

E.2 MACHINE LEARNING FOR CODE OPTIMIZATION

Machine learning (ML) has emerged as a powerful tool to transcend the limitations of hand-crafted heuristics. Early work focused on using ML to make better decisions within existing compiler and tuning frameworks. Systems like TVM employ a learned cost model to predict the performance of kernel variants, guiding the search process and avoiding exhaustive empirical evaluation (Chen et al., 2018). More recent efforts have integrated ML directly into production compilers. Google’s MLGO framework uses reinforcement learning (RL) to train policies for classic compiler optimizations like function inlining and register allocation, demonstrating significant improvements in code size and performance over decades-old, manually-tuned heuristics in LLVM (Trofin et al., 2021; Marinov

```

810
811 1 ## System Message
812
813 2 You are a GPU kernel engineer tasked with accelerating a PyTorch
814 3 model by selectively replacing its operators with custom CUDA
815 4 kernels.
816 5 You have full discretion in deciding which operators should be
817 6 rewritten, fused, or left as-is. You may implement multiple custom
818 7 kernels, explore operator fusion (e.g., matmul + activation), or
819 8 introduce more efficient algorithmic variants (such as online
820 9 softmax or tiled reductions).
821
822 10 Your design space is unrestricted creativity and performance
823 11 intuition should guide your choices.
824
825 12 Whenever beneficial, leverage CUDA's high-performance primitives (
826 13 tensor cores, cutlass, cuBLAS, cuDNN, etc.). Build upon these
827 14 optimized components and push performance further with your own
828 15 implementations.
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Figure 7: Alternate System Message V2 for STARK.

et al., 2024). These models can learn from massive code corpora and discover complex feature interactions that are opaque to human experts (Cummins et al., 2017).

A more profound application of ML has been in algorithmic discovery. DeepMind’s AlphaTensor framed the search for faster matrix multiplication algorithms as a single-player game, using a deep RL agent based on AlphaZero to navigate the enormous search space of tensor decompositions (Fawzi et al., 2022). This approach successfully discovered novel, provably correct algorithms that outperform human-derived state-of-the-art methods, including improving upon Strassen’s algorithm for 4×4 matrices for the first time in over 50 years (Fawzi et al., 2022; DeepMind, 2022). This work marked a critical shift from using ML to *configure* existing optimization strategies to using it to *invent* new ones from first principles. However, AlphaTensor operated in a clean, formal mathematical domain. Translating this power to the messy, syntactic, and hardware-constrained domain of GPU kernel programming presents a distinct challenge. Our work addresses this by employing an agent that operates directly on source code, navigating the complexities of syntax, compilation, and hardware-specific performance characteristics.

E.3 LLM-POWERED AUTONOMOUS AGENTS

The capabilities of LLMs have given rise to a new paradigm of autonomous agents. An LLM agent uses a core LLM as its “brain” or controller, augmented with capabilities for planning, memory, and tool use to perform complex tasks autonomously (Weng, 2023). The key distinction from simple LLM prompting is the agent’s ability to decompose a high-level goal into a sequence of manageable subtasks, execute them iteratively, and use reflection to gauge progress and self-correct. This agentic workflow involves the LLM interacting with an external environment through a set of tools, such as a code interpreter or a web search API, to gather information and perform actions. While this paradigm is powerful for general problem-solving, its application to specialized domains like software engineering requires tailored tools and reasoning processes. Our work specializes this agentic concept for the domain of performance optimization, which presents unique challenges not found in general-purpose agent tasks.

E.4 LLMs FOR CODE OPTIMIZATION AND GENERATION

The advent of powerful LLMs has opened a new frontier in performance engineering. To grant LLMs greater autonomy, the agentic paradigm has been adapted specifically for software engineering. The success of systems like SWE-agent, which autonomously resolves complex bugs in large GitHub repositories, has demonstrated the viability of this approach (Yang et al., 2024). SWE-agent equips an LLM with a specialized Agent-Computer Interface (ACI) containing tools for file navigation, editing, and test execution, enabling it to perform long-horizon tasks far beyond the scope of

```

864 1 ## Instruction
865 2
866 3 - Optimize the architecture named Model with custom CUDA operators
867 4 !
868 5 - Give explicit and actionable advice to improve the efficiency, in
869 6 terms of the GPU wall-clock time, of the architecture named Model
870 7 .
871 8
872 9 - Give ONE advice of the top priority! Don't over-request.
873 10 - Include necessary details such as how to change pointers and
874 11 indices or how to achieve shared memory tiling so that your advice
875 12 can be correctly implemented.
876 13
877 14 - After your advice, modify and return the given source code in
878 15 the following way:
879 16     - Identify the code block whose efficiency can be improved ( that
880 17 is where your advice should be implemented)
881 18     and mark it with comments '<<<IMPROVE BEGIN>>>' at the
882 19 beginning and '<<<IMPROVE END>>>' at the end
883 20     - The markers '<<<IMPROVE BEGIN>>>' and '<<<IMPROVE END>>>' should be valid comments for the marked coding language. For
884 21 example, when marking source code of custom kernels, you need to
885 22 use comments for the C++ language as '/* <<<IMPROVE BEGIN>>>*/' and
886 23 '/* <<<IMPROVE END>>>*/'; when marking source code of Python, you
887 24 should use '# # <<<IMPROVE BEGIN>>>' and '# # <<<IMPROVE END>>>'.
888 25     - Add your advice as comments at the identified code block to
889 26 help the following agent's implementation
890 27     - There will be another agent focusing on improving the
891 28 efficiency of the identified code block.
892 29     - Return the complete code block with the identified code
893 30 block as its subpart.
894 31
895 32     - You should consider using CUDA's existing highly optimized
896 33 kernels and operations whenever appropriate. Try building on these
897 34 optimized blocks and further improve it with your custom kernels.
898 35     - When presented with multiple prior attempts, you should consider
899 36 exploration of more diverse optimization strategies.
900 37     - Pay careful attention to the implementation agent's capability
901 38 demonstrated from the historical implementations.
902 39     - Adjust your advice accordingly to ensure that it can
903 40 successfully implement.
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Figure 8: Instruction for the Plan Agent.

simple code generation (Yang et al., 2024; Jimenez et al., 2024). While these agents are a significant step towards autonomous software engineering, their focus has primarily been on functional correctness, such as bug fixing. Our work extends this agentic software engineering paradigm to the non-functional, performance-oriented domain of GPU kernel optimization. We introduce an agent that not only interacts with a codebase but also with hardware profiling tools, allowing it to autonomously diagnose performance bottlenecks, form hypotheses, and conduct experiments to iteratively improve kernel efficiency, thus acting as a true autonomous performance engineer.

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1 ## Instruction
2
3 Optimize the architecture named Model with custom CUDA operators!
4
5 - Think about the given advice from human experts and implement
6 the ones that you believe are correct and you are confident
7 implementing.
8 - Only focus on the code block marked with '<<<IMPROVE BEGIN>>>' and '<<<IMPROVE END>>>'
9 - Write custom cuda kernel to replace the pytorch operators within
10 the marked code block to improve its efficiency
11 - Name your optimized output architecture ModelNew.
12 - Output the new code in codeblocks.
13 - Explain your implementation and how you follow the advice.
14 - Using the given tool to return your final structured answer.
15 Please generate real code, NOT pseudocode, make sure the code
16 compiles and is fully functional.
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18 NO testing code!
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Figure 9: Instruction for the Code Agent.

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1 ## Instruction
2
3 Fix the issues of your implementation named ModelNew, which should
4 improve efficiency of the source model named Model.
5
6 - ModelNew and Model should have the same functionality, that is,
7 the same input-output mapping.
8 - The given architecture ModelNew either does not compile, or has
9 run-time error, or has different functionality to the source
10 Model.
11 - Use the given observations to infer bugs and then fix them.
12 - Explain how the bugs happen and how you fix it.
13 - Return the fixed bug-free code and name your optimized output
14 architecture ModelNew.
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Figure 10: Instruction for the Debug Agent.

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986
987     ## Example Architecture Source Code
988 1  import torch
989 2  import torch.nn as nn
990 3  import torch.nn.functional as F
991 4
992 5
993 6
994 7 class Model(nn.Module):
995 8     def __init__(self) -> None:
996 9         super().__init__()
997 10
998 11     def forward(self, a, b):
999 12         return a + b
1000 13
1001 14
1002 15     def get_inputs():
1003 16         # randomly generate input tensors based on the model
1004 17         architecture
1005 18         a = torch.randn(1, 128).cuda()
1006 19         b = torch.randn(1, 128).cuda()
1007 20         return [a, b]
1008 21
1009 22     def get_init_inputs():
1010 23         # randomly generate tensors required for initialization based
1011 24         on the model architecture
1012 25         return []
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Figure 11: In-context Example Architecture for All Agents.

```

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1028     1 ## Example New Architecture Source Code
1029
1030     2 import torch
1031     3 import torch.nn as nn
1032     4 import torch.nn.functional as F
1033     5 from torch.utils.cpp_extension import load_inline
1034
1035     6 # Define the custom CUDA kernel for element-wise addition
1036     7 elementwise_add_source = """
1037     8 #include <torch/extension.h>
1038     9 #include <cuda_runtime.h>
1039
1040    10 __global__ void elementwise_add_kernel(const float* a, const float
1041    11 * b, float* out, int size) {
1042    12     int idx = blockIdx.x * blockDim.x + threadIdx.x;
1043    13     if (idx < size) {
1044    14         out[idx] = a[idx] + b[idx];
1045    15     }
1046    16 }
1047
1048    17 torch::Tensor elementwise_add_cuda(torch::Tensor a, torch::Tensor
1049    18 b) {
1050    19     auto size = a.numel();
1051    20     auto out = torch::zeros_like(a);
1052
1053    21     const int block_size = 256;
1054    22     const int num_blocks = (size + block_size - 1) / block_size;
1055
1056    23     elementwise_add_kernel<<<num_blocks, block_size>>>(a.data_ptr<
1057    24 float>(), b.data_ptr<float>(), out.data_ptr<float>(), size);
1058
1059    25     return out;
1060    26 }
1061    27 """
1062
1063    28 elementwise_add_cpp_source = (
1064    29     "torch::Tensor elementwise_add_cuda(torch::Tensor a, torch::
1065    30 Tensor b);"
1066    31 )
1067
1068    32 # Compile the inline CUDA code for element-wise addition
1069    33 elementwise_add = load_inline(
1070    34     name="elementwise_add",
1071    35     cpp_sources=elementwise_add_cpp_source,
1072    36     cuda_sources=elementwise_add_source,
1073    37     functions=["elementwise_add_cuda"],
1074    38     verbose=True,
1075    39     extra_cflags=[],
1076    40     extra_ldflags=[],
1077    41 )
1078
1079    42 class ModelNew(nn.Module):
1080    43     def __init__(self) -> None:
1081    44         super().__init__()
1082    45         self.elementwise_add = elementwise_add
1083
1084    46     def forward(self, a, b):
1085    47         return self.elementwise_add.elementwise_add_cuda(a, b)

```

Figure 12: In-context Optimized Example Architecture for All Agents.

```

1080
1081
1082
1083
1084
1085
1086
1087
1088
1089
1090
1091
1092     1 import torch
1093     2 import torch.nn as nn
1094
1095     3
1096     4 class Model(nn.Module):
1097         5     """
1098             6     Simple model that performs a LogSoftmax activation.
1099         7     """
1100         8     def __init__(self, dim: int = 1):
1101             9         super(Model, self). __init__()
1102             10        self.dim = dim
1103
1104         11
1105         12     def forward(self, x: torch.Tensor) -> torch.Tensor:
1106             13         """
1107                 14             Applies LogSoftmax activation to the input tensor.
1108             15
1109             16             Args:
1110                 17                 x (torch.Tensor): Input tensor of shape (batch_size, dim).
1111
1112             18
1113             19             Returns:
1114                 20                 torch.Tensor: Output tensor with LogSoftmax applied, same shape as input.
1115             21             """
1116             22         return torch.log_softmax(x, dim=self.dim)
1117
1118             23
1119             24         batch_size = 4096
1120             25         dim = 393216
1121
1122             26
1123             27         def get_inputs():
1124                 28             x = torch.rand(batch_size, dim)
1125                 29             return [x]
1126
1127             30
1128             31         def get_init_inputs():
1129                 32             return [] # No special initialization inputs needed
1130
1131
1132
1133

```

Figure 13: Example KernelBench Level 1 Task.

```
1134
1135
1136
1137
1138
1139
1140
1141
1142
1143
1144 1 import torch
1145 2 import torch.nn as nn
1146 3
1147 4 class Model(nn.Module):
1148 5     """
1149 6         Model that performs a matrix multiplication, division,
1150 7             summation, and scaling.
1151 8     """
1152 9     def __init__(self, input_size, hidden_size, scaling_factor):
115310         super(Model, self).__init__()
115411         self.weight = nn.Parameter(torch.randn(hidden_size,
115512             input_size))
115613         self.scaling_factor = scaling_factor
115714
115815     def forward(self, x):
115916         """
116017             Args:
116118                 x (torch.Tensor): Input tensor of shape (batch_size,
116219                 input_size).
116320             Returns:
116421                 torch.Tensor: Output tensor of shape (batch_size,
116522                 hidden_size).
116623         """
116724         x = torch.matmul(x, self.weight.T)    # Gemm
116825         x = x / 2    # Divide
116926         x = torch.sum(x, dim=1, keepdim=True) # Sum
117027         x = x * self.scaling_factor    # Scaling
117128         return x
117229
117330         batch_size    = 1024
117431         input_size    = 8192
117532         hidden_size   = 8192
117633         scaling_factor = 1.5
117734
117835     def get_inputs():
117936         return [torch.rand(batch_size, input_size)]
118037
118138     def get_init_inputs():
118239         return [input_size, hidden_size, scaling_factor]
```

Figure 14: Example KernelBench Level 2 Task.

```

1188 1 import torch
1189 2 import torch.nn as nn
1190 3 import torch.nn.functional as F
1191 4 import math
1192 5
1193 6 class NewGELU(nn.Module):
1194 7     """
1195 8     Implementation of the GELU activation function currently in
1196 9     Google BERT repo (identical to OpenAI GPT).
1197 10    Reference: Gaussian Error Linear Units (GELU) paper: https://arxiv.org/abs/1606.08415
1198 11    """
1199 12    def __init__(self):
1200 13        super(NewGELU, self).__init__()
1201 14
1202 15    def forward(self, x):
1203 16        return 0.5 * x * (1.0 + torch.tanh(math.sqrt(2.0 / math.pi)
1204 17            ) * (x + 0.044715 * torch.pow(x, 3.0)))
1205 18
1206 19 class CausalSelfAttention(nn.Module):
1207 20     """
1208 21     A vanilla multi-head masked self-attention layer with a
1209 22     projection at the end.
1210 23     It is possible to use torch.nn.MultiheadAttention here but I
1211 24     am including an
1212 25     explicit implementation here to show that there is nothing too
1213 26     scary here.
1214 27     """
1215 28
1216 29    def __init__(self, n_embd, n_head, attn_pdrop, resid_pdrop,
1217 30        max_seqlen):
1218 31        super().__init__()
1219 32        assert n_embd % n_head == 0
1220 33        # key, query, value projections for all heads, but in a
1221 34        # batch
1222 35        self.c_attn = nn.Linear(n_embd, 3 * n_embd)
1223 36        # output projection
1224 37        self.c_proj = nn.Linear(n_embd, n_embd)
1225 38        # regularization
1226 39        self.attn_dropout = nn.Dropout(attn_pdrop)
1227 40        self.resid_dropout = nn.Dropout(resid_pdrop)
1228 41        # causal mask to ensure that attention is only applied to
1229 42        # the left in the input sequence
1230 43        self.register_buffer("bias", torch.tril(torch.ones(
1231 44            max_seqlen, max_seqlen))
1232 45            .view(1, 1, max_seqlen,
1233 46            max_seqlen))
1234 47        self.n_head = n_head
1235 48        self.n_embd = n_embd
1236 49        [...skipped]
1237 50
1238 51 class Model(nn.Module):
1239 52     """
1240 53     an unassuming Transformer block """
1241 54
1242 55    [...skipped]
1243 56
1244 57    def forward(self, x):
1245 58        x = x + self.attn(self.ln_1(x))
1246 59        x = x + self.mlpf(self.ln_2(x))
1247 60        return x
1248 61
1249 62    [...skipped]

```

Figure 15: Example KernelBench Level 3 Task.