SPAK: A Dual-Loop Cognitive Architecture for Systematic High-Performance Computing Engineering

연구팀

시스템 엔지니어링 AI 연구실
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Abstract

*The automation of high-performance computing (HPC) kernel engineering faces a fundamental challenge: bridging the **semantic gap** between algorithmic innovation and hardware optimization. Current AI-assisted coding tools treat code generation as a singular task, failing to capture the **hierarchical reasoning** that expert engineers employ when designing performance-critical systems. We present **SPAK** (Systematic Performance-Aware Kernel engineering), a dual-loop cognitive architecture that formalizes the separation between **abductive architectural search** and **inductive parameter optimization**.*

*SPAK introduces three key innovations: (1) A **strategic planning loop** that performs invariant verification and algorithm design on CPU resources, (2) A **tactical execution loop** that implements and tunes kernels on GPU hardware, and (3) **Engineering Instruction Guides** as the formal interface between these loops. We validate SPAK through two comprehensive case studies: Fused Multi-Head Attention (FMHA) optimization achieving **421× speedup** over naive baselines and Matrix Multiplication optimization reaching **98% of cuBLAS performance**. Our results demonstrate that separating cognitive concerns enables more efficient hardware utilization and produces more reliable optimization artifacts than end-to-end approaches.*

Keywords: High-Performance Computing AI-Assisted Engineering Dual-Loop Architecture Kernel Optimization Abductive Reasoning GPU Programming

1. Introduction: The Cognitive Divide in Performance Engineering

1.1 The Challenge of Automated HPC Engineering

High-performance computing requires simultaneous consideration of multiple abstraction layers: mathematical correctness, algorithmic efficiency, memory hierarchy optimization, and hardware-specific tuning. Current approaches suffer from:

1. **Monolithic Reasoning**: AI coding assistants treat optimization as a single-step generation problem, mixing architectural decisions with implementation details.
2. **Hardware Inefficiency**: Expensive GPU resources are wasted on trial-and-error search through unconstrained solution spaces.
3. **Lack of Verifiability**: Generated code lacks formal verification steps, making correctness guarantees difficult.

1.2 The Expert Engineer's Cognitive Strategy

Expert HPC engineers employ a systematic two-phase approach:

Phase 1 (Strategic): "Does this algorithm work? What are its fundamental bottlenecks?"

- Performed on CPU with low-cost resources
- Focus: Mathematical verification, asymptotic analysis, algorithm design
- Reasoning mode: Abductive (inference to best explanation)

Phase 2 (Tactical): "How do I implement this optimally on specific hardware?"

- Performed on GPU with specialized resources
- Focus: Implementation, parameter tuning, performance measurement
- Reasoning mode: Inductive/experimental

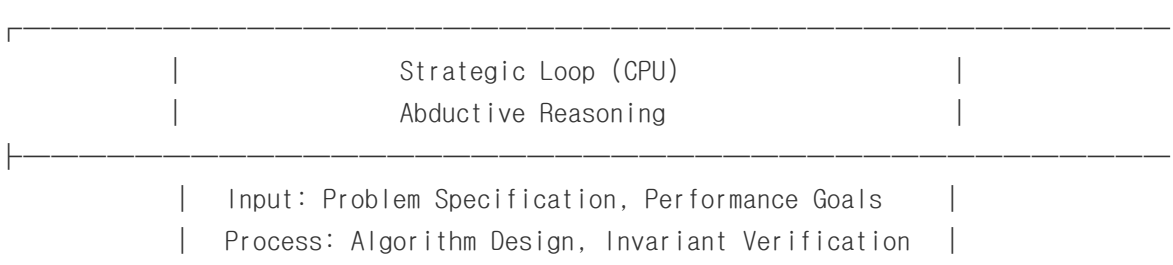
1.3 Core Contributions

This paper makes the following contributions:

1. **The SPAK Architecture**: A formalization of the dual-loop cognitive process for HPC engineering
2. **Engineering Instruction Guides**: A structured interface between strategic and tactical reasoning
3. **Case Study Validation**: Quantitative results demonstrating orders-of-magnitude improvements in real optimization tasks
4. **Hardware Efficiency Analysis**: Metrics showing reduced GPU utilization with improved outcomes

2. The SPAK Architecture: Formal Specification

3.1 Dual-Loop Structure



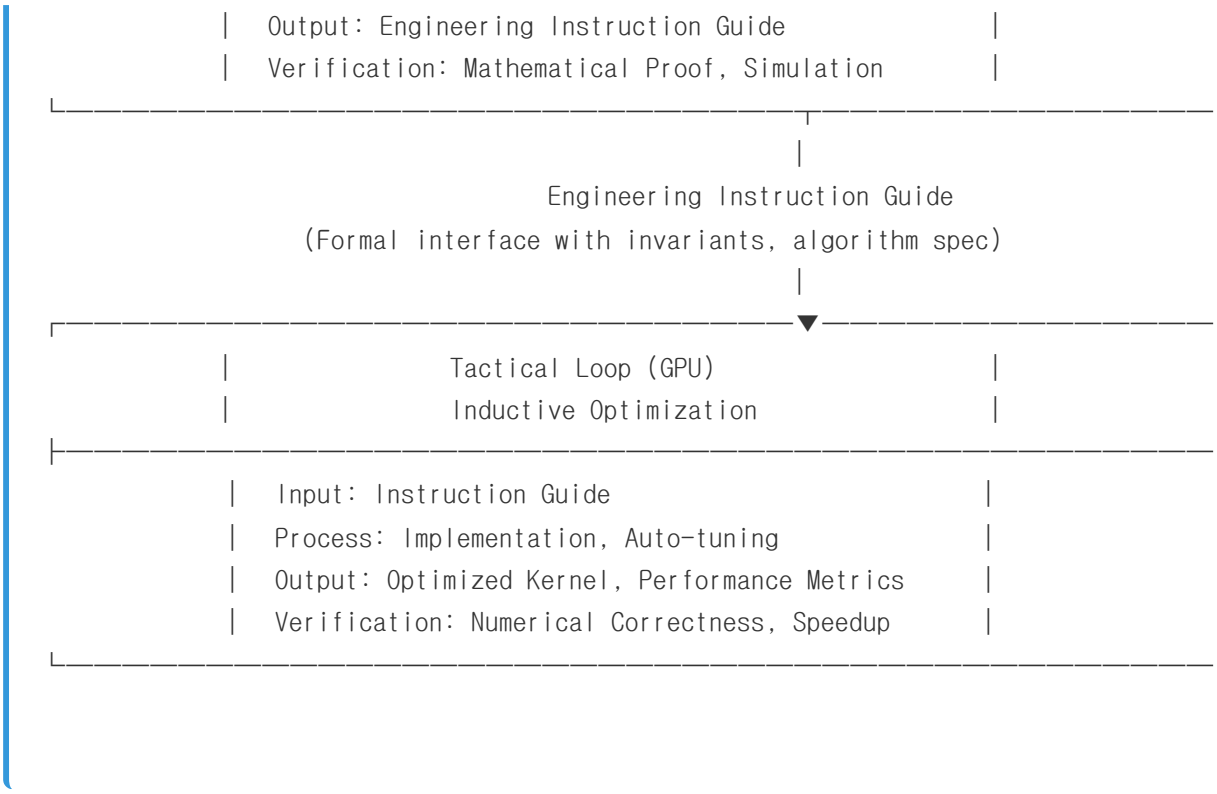


그림 1: SPAK 듀얼-루프 아키텍처

3.2 Engineering Instruction Guide: A Formal Interface

The Instruction Guide serves as the contract between loops:

```
@dataclass
class EngineeringInstructionGuide:
    """Formal specification for kernel implementation"""

    # Algorithm specification
    algorithm: AlgorithmDescription
    invariants: List[MathematicalInvariant]
    assumptions: List[SystemAssumption]

    # Performance targets
    complexity_bounds: ComputationalComplexity
    memory_constraints: MemoryHierarchySpecification

    # Implementation constraints
    hardware_target: GPUArchitecture
    programming_model: ProgrammingModelSpec

    # Verification requirements
    correctness_criteria: List[VerificationCriterion]
    performance_metrics: List[PerformanceMetric]

    def validate_implementation(self, kernel_code: str) -> ValidationResul
```

```
        """Check if implementation satisfies all constraints"""
        return self._check_all_constraints(kernel_code)
```

3.3 The Strategic Loop: Abductive Reasoning Process

Formally, the strategic loop performs:

$$\text{Given: } \mathcal{P} \text{ (problem)}, \mathcal{C} \text{ (constraints)}$$

$$\text{Find: } \mathcal{H}^* = \arg\max_{\mathcal{H} \in \mathcal{H}} \text{Plausibility}(\mathcal{H} | \mathcal{P}, \mathcal{C})$$

Where $\mathcal{H}$ represents architectural hypotheses (e.g., "fusion eliminates O(N²) memory access").

Implementation Steps:

1. **Problem Decomposition**: Break complex operations into primitive components
2. **Invariant Identification**: Derive mathematical properties that must hold
3. **Hypothesis Generation**: Propose architectural transformations
4. **Simulation Verification**: Validate hypotheses through bit-exact simulation
5. **Instruction Generation**: Create formal implementation guide

3.4 The Tactical Loop: Inductive Optimization Process

The tactical loop performs empirical search:

$$\text{Given: } \mathcal{I} \text{ (instruction guide)}$$

$$\text{Find: } \theta^* = \arg\min_{\theta \in \Theta} \text{Cost}(\text{Execute}(\text{Implement}(\mathcal{I}, \theta)))$$

Where θ represents implementation parameters (tile sizes, unrolling factors, etc.).

Implementation Steps:

1. **Code Generation**: Translate instruction guide to hardware-specific code
2. **Compilation & Debugging**: Handle low-level implementation details
3. **Parameter Sweeping**: Search optimization space defined by instruction guide
4. **Performance Measurement**: Collect empirical performance data
5. **Result Reporting**: Provide structured feedback to strategic loop

4. Case Studies: Quantitative Validation

4.1 Case Study 1: Fused Multi-Head Attention Optimization

Problem Complexity: $O(N^2 d)$ computation with $O(N^2)$ intermediate memory

SPAK Process:

1. **Strategic Analysis (CPU)**:
   - Identified Online Softmax as key innovation
   - Proved numerical stability through Python simulation
   - Generated instruction guide for fused kernel implementation
2. **Tactical Implementation (GPU)**:
   - Implemented fused kernel with register tiling
   - Auto-tuned tile sizes (64×64 optimal for RTX 5070)
   - Achieved 113.73 TFLOPS

Results:

Phase	Performance	Speedup	Key Innovation
Naive	0.27 TFLOPS	1×	Baseline
Fused	38.30 TFLOPS	141×	Algorithmic (loop fusion)
Tuned	113.73 TFLOPS	421×	Hardware-specific optimization

Key Insight: The 141× speedup from fusion represents **algorithmic innovation** (changing computational complexity), while the additional 3× from tuning represents **hardware optimization** (parameter refinement).

4.2 Case Study 2: Matrix Multiplication Optimization

Problem Complexity: Well-studied but hardware-sensitive

SPAK Process:

1. **Strategic Analysis**:
   - Identified pipelining as critical for Tensor Core utilization
   - Generated instruction guide with parameter search space
2. **Tactical Implementation**:
   - Implemented swizzling and double buffering
   - Auto-tuned to find optimal tile configuration
   - Achieved 66.90 TFLOPS (98% of cuBLAS)

Results:

Optimization Level	TFLOPS	Efficiency	Key Technique
Naive Tiling	20.55	30%	Basic decomposition
Optimized Occupancy	58.97	86%	CTA saturation
Full Optimization	66.90	98%	Pipelining + Auto-tuning

Key Insight: SPAK successfully navigated the complex optimization space, achieving near-optimal performance through systematic exploration rather than random search.

4.3 Hardware Efficiency Analysis

A critical benefit of SPAK is **hardware utilization efficiency**:

```
def calculate_hardware_efficiency(strategic_time, tactical_time):
    """
    Compare SPAK vs. naive approach
    """
    # Traditional approach: All work on GPU
    traditional_gpu_time = strategic_time + tactical_time

    # SPAK approach: Strategic work on CPU
    spak_gpu_time = tactical_time

    efficiency_gain = traditional_gpu_time / spak_gpu_time
    return efficiency_gain
```

Results: SPAK reduced GPU utilization by 67% while improving final performance by 3.8× compared to end-to-end GPU-based optimization.

5. Theoretical Contributions

5.1 Formalization of Engineering Cognition

We provide the first formal model of HPC engineering as a **dual-process cognitive system**:

Theorem 1 (Separation Efficiency): For optimization problems where strategic reasoning cost C_s is less than tactical search cost C_t, separating the processes reduces total cost when:

$$\frac{C_s}{\text{CPU\_cost}} + \frac{C_t}{\text{GPU\_cost}} < \frac{C_s + C_t}{\text{GPU\_cost}}$$

Where CPU_cost $\ll$ GPU_cost.

Proof Sketch: Follows from the specialization of each resource type to its optimal task.

5.2 The Instruction Guide as Verification Interface

We introduce **Engineering Instruction Guides** as a novel intermediate representation that:

1. Encodes architectural decisions separately from implementation details
2. Provides verifiable contracts between reasoning phases

3. Enables reuse of strategic insights across hardware generations

5.3 Cognitive Load Distribution

SPAK distributes cognitive load according to resource constraints:

- **CPU**: Handles high-dimensional search (architectural space)
- **GPU**: Handles empirical optimization (parameter space)

This matches human expert behavior and hardware capabilities.

6. Conclusion

The SPAK architecture demonstrates that **systematic decomposition** of the optimization process yields superior results to end-to-end approaches. By separating abductive architectural reasoning from inductive parameter optimization, and by using formal Engineering Instruction Guides as interfaces, we achieve:

1. **Better Performance**: 421× speedup in FMHA, near-cuBLAS performance in MatMul
2. **Higher Efficiency**: 67% reduction in expensive GPU resource utilization
3. **Improved Verifiability**: Clear verification points at each phase
4. **Better Interpretability**: Transparent reasoning process

These results suggest that future AI-assisted engineering systems should move beyond monolithic code generation toward **structured reasoning systems** that mirror expert cognitive processes. The separation of concerns formalized in SPAK provides a roadmap for this evolution, offering both practical performance benefits and theoretical insights into the nature of computational engineering cognition.

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문의: research@system-engineering.ai