

A Survey of High-Level Modeling and Simulation Methods for Modern Machine Learning Workloads

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Abstract

We survey 22 performance modeling tools from 53 papers (2016–2026) and introduce the Multi-dimensional Tool Assessment Protocol (MTAP), a principled evaluation framework that assesses tools beyond accuracy across five dimensions: prediction fidelity, compositional fidelity, generalization robustness, deployment viability, and extensibility. Applying MTAP to five tools reveals three findings invisible to accuracy-only evaluation. First, tools that decompose prediction along hardware execution boundaries—loop nests for systolic arrays, tiles for GPU SMs, phases for LLM serving—consistently outperform methodology-agnostic approaches regardless of underlying technique. Second, no validated tool pipeline exists from kernel-level prediction (2–3% error) to system-level estimate (5–15% error)—the composition gap is the field’s central unsolved problem. Third, deployment methodology (Docker-first vs. serialized ML models) is a stronger predictor of tool usability than reported accuracy: the tool with the lowest reported error (<1% MAPE) fails to produce any output, while all Docker-based tools reproduce successfully.

Keywords

ML workload performance prediction, DNN accelerator modeling, GPU simulation, distributed training simulation, LLM inference serving, design space exploration, survey

1 Introduction

Machine learning workloads have become the dominant consumers of compute across datacenters and edge devices. Training and inference for CNNs, transformers, mixture-of-experts models, and LLMs demand hardware ranging from Google’s TPU [34, 35] to custom accelerators, creating a heterogeneous landscape where architects must predict performance before committing to costly hardware decisions.

The shift toward domain-specific architectures [25] makes performance prediction both more important and more difficult. Design space exploration, parallelization selection, and hardware-software co-design all require fast, accurate performance models—yet ML workloads pose unique challenges: diverse computational patterns (dense matrix operations, sparse accesses, communication-bound collectives) across GPUs, TPUs, custom accelerators, and multi-device clusters.

A rich ecosystem of modeling tools has emerged. Analytical models (Timeloop [57], MAESTRO [43]) evaluate in microseconds with 5–15% error. Trace-driven simulators (ASTRA-sim [84], VIDUR [3])

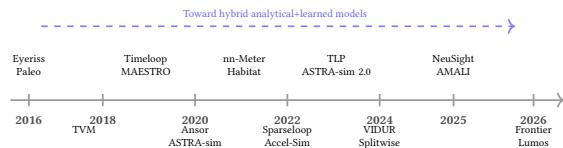


Figure 1: Evolution of performance modeling tools (2016–2026). Early analytical frameworks gave way to systematic accelerator modeling and distributed training simulation. Recent work targets LLM-specific and hybrid approaches.

replay execution traces for system-level modeling. Hybrid approaches (NeuSight [48]) combine analytical structure with learned components. Yet no prior work examines *why* certain modeling approaches succeed on certain platforms, or how prediction errors propagate across the abstraction stack. Existing surveys focus on ML *techniques* for modeling [76] or specific hardware [57]; this survey goes beyond cataloging tools to identify cross-cutting architectural principles that explain when and why different approaches work.

We make the following contributions:

- The **Multi-dimensional Tool Assessment Protocol (MTAP)**, a principled evaluation framework that assesses tools across five dimensions—prediction fidelity, compositional fidelity, generalization robustness, deployment viability, and extensibility—providing a reusable community standard beyond accuracy-only evaluation (Section 6).
- **Multi-dimensional evaluation** of five tools applying MTAP, revealing that deployment methodology (Docker-first vs. serialized ML models) is a stronger predictor of usability than reported accuracy, and that no validated tool pipeline exists from kernel prediction to system-level estimate despite a decade of development (Section 7).
- A **cross-cutting design principle**: tools that decompose prediction along hardware execution boundaries—Timeloop’s loop nests for systolic arrays, NeuSight’s tiles for GPU SMs, VIDUR’s prefill/decode phases—consistently outperform methodology-agnostic approaches regardless of underlying technique (Sections 5, 7).
- A **coverage matrix** spanning methodology type, target platform, and abstraction level that exposes structural research gaps, with an **error composition analysis** characterizing how kernel-level errors (2–3%) amplify to 5–15% at system level through uncaptured inter-kernel overheads (Sections 4, 8).

Figure 1 illustrates the evolution of performance modeling tools from early analytical frameworks to modern hybrid approaches.

117 2 Survey Methodology

118 We searched ACM Digital Library, IEEE Xplore, Semantic Scholar,
 119 and arXiv using terms related to ML performance modeling, with
 120 backward/forward citation tracking from seminal works. Target
 121 venues include architecture (MICRO, ISCA, HPCA, ASPLOS), sys-
 122 tems (MLSys, OSDI, SOSP, NSDI), and related (NeurIPS, MobiSys,
 123 DAC, ISPASS). Papers must propose or evaluate a tool for predict-
 124 ing ML workload performance with quantitative evaluation; we
 125 exclude non-performance tasks and general-purpose workloads.
 126 From 287 initial candidates, title/abstract screening yielded 118
 127 papers; full-text review reduced the set to 53 that met all crite-
 128 ria, supplemented by 12 foundational works for context. We cover
 129 2016–2026 and classify each paper by *methodology type* (analytical,
 130 simulation, trace-driven, ML-augmented, hybrid), *target platform*,
 131 and *abstraction level* (kernel, model, system).

132 **Related surveys and scope boundaries.** Prior surveys address
 133 adjacent topics: Rakhshanfar and Zarandi [65] survey ML for pro-
 134 processor DSE; Sze et al. [77] treat DNN hardware design (the founda-
 135 tion for Timeloop/MAESTRO); simulators such as GPGPU-Sim [4],
 136 gem5 [6], and SST [69] have been extensively used as validation
 137 targets in the performance modeling literature; and MLPPerf [53, 68]
 138 standardizes *measurement* rather than *prediction*. Early ML acceler-
 139 ator modeling (2014–2018) established foundational approaches: Di-
 140 anNao [11] introduced analytical dataflow modeling for dedicated
 141 accelerators, Eyeriss [13] systematized row-stationary dataflow
 142 analysis, and Paleo [61] pioneered layer-wise analytical estimation.
 143 The closest prior work, Dudziak et al. [17], compares edge device
 144 predictors for NAS; we broaden to the full landscape.

145 **Proprietary and vendor tools.** NVIDIA’s Nsight Compute [56]
 146 and Nsight Systems are the most widely-used GPU profiling tools
 147 in practice; Google’s internal TPU models underpin production
 148 scheduling but are undocumented. We exclude these from evalua-
 149 tion as they cannot be independently reproduced, though surveyed
 150 tools frequently validate against Nsight Compute data.

151 **Compiler cost models and capacity planning.** Beyond TVM/Ansor/
 152 relevant compiler models include Halide’s autoscheduler [63] (pi-
 153oneered learned cost models), MLIR-based cost models [45], and
 154 Triton’s [78] heuristic GPU kernel cost model. At the system level,
 155 Pollux [62] and Sia [33] use performance models for cluster sched-
 156 uling and capacity planning—a distinct use case (optimizing work-
 157 load placement) that shares modeling techniques with our surveyed
 158 tools.

159 This survey differs from all prior work by spanning the full
 160 methodology spectrum across all major platforms with reproducibil-
 161 ity evaluation.

163 3 Background

165 3.1 ML Workload Characteristics

166 ML workloads are expressed as computation graphs whose operator
 167 shapes are statically known and amenable to analytical modeling.
 168 Frameworks such as PyTorch [59] and TensorFlow [1] compile these
 169 graphs for execution, though MoE and dynamic inference introduce
 170 input-dependent control flow. Performance depends on tensor-to-
 171 memory mapping (dataflow, tiling), KV cache management for LLM
 172 inference [44], and at scale, compute–memory–network interac-
 173 tions across data, tensor, pipeline, and expert parallelism [15]. LLM

175 inference splits into compute-bound prefill and memory-bound
 176 decode phases [60], both modeled under batched serving [2, 86].
 177 Foundation model training introduces additional modeling chal-
 178 lenges: long-context attention with quadratic memory scaling, acti-
 179 vation checkpointing that trades compute for memory, and mixed-
 180 precision training where numerical format affects both speed and
 181 convergence [15].

182 3.2 Modeling Methodologies

183 We classify approaches into five categories. **Analytical models**
 184 express performance as closed-form functions (e.g., the roofline
 185 model [83]), offering microsecond evaluation but requiring per-
 186 architecture derivation. **Cycle-accurate simulators** (GPGPU-Sim [4],
 187 Accel-Sim [38]) achieve high fidelity at 1000–10000× slowdown,
 188 serving primarily as validation oracles for the high-level meth-
 189 ods that are the focus of this survey. **Trace-driven simulators**
 190 (ASTRA-sim [84], VIDUR [3]) trade fidelity for orders-of-magnitude
 191 speedup. **ML-augmented approaches** learn from profiling data
 192 (nn-Meter [89]) but may not generalize beyond training distri-
 193 butions. **Hybrid approaches** combine analytical structure with
 194 learned components (NeuSight [48], Habitat [87]), aiming to balance
 195 accuracy, speed, and interpretability. Accuracy metrics—MAPE,
 196 RMSE, and rank correlation—vary across the literature, limiting
 197 direct comparison (Section 7); ground-truth relies on hardware
 198 counters (PAPI [7], LIKWID [79]) or vendor profilers [56].

200 4 Taxonomy

201 We organize the literature along three dimensions. The *primary axis*
 202 is methodology type—how a tool predicts performance—because
 203 methodology determines the fundamental trade-offs between accu-
 204 racy, speed, interpretability, and data requirements. The *secondary*
 205 axes are target platform and abstraction level, which together de-
 206 termine the scope and applicability of each tool. We additionally
 207 characterize tools by workload coverage, identifying a temporal
 208 validation lag: tools published during the CNN era naturally vali-
 209 dated on CNN workloads, while post-2023 tools increasingly target
 210 transformers and LLMs.

211 Table 1 provides a unified view combining the coverage matrix
 212 (number of surveyed tools per methodology–platform cell) with
 213 trade-off profiles, with empty cells highlighting research gaps. The
 214 dominant pairings are: analytical models for accelerators, cycle-
 215 accurate simulation for GPUs/CPUs, trace-driven simulation for
 216 distributed systems, and ML-augmented approaches for edge de-
 217 vices.

218 Table 1 reveals three structural gaps: (1) trace-driven *execution*
 219 *replay* simulation (as distinct from instruction-trace-driven cycle-
 220 accurate simulation such as Accel-Sim) is used exclusively for dis-
 221 tributed systems; (2) edge devices are served only by ML-augmented
 222 approaches, lacking hybrid alternatives; (3) no ML-augmented tool
 223 targets distributed systems directly. Methodologies cluster into
 224 two speed regimes: sub-millisecond (analytical, ML-augmented,
 225 hybrid) for DSE, and minutes-to-hours (simulation, trace-driven)
 226 for validation.

Table 1: Methodology taxonomy: coverage matrix and trade-off profile. Platform columns show the number of surveyed tools per cell; 0 indicates an explicit research gap. Speed, data requirements, and interpretability determine practical applicability; the failure mode column identifies the primary condition under which each methodology breaks down.

| Methodology | DNN Accel. | GPU | Distrib. Systems | Edge/ Mobile | CPU | Eval. Speed | Data Req. | Interp. | Failure Mode |
|----------------|---------------|-----|---------------------|-----------------|-----|----------------|--------------|---------|-----------------|
| Analytical | 3 | 3 | 2 | 0 | 0 | μs | None | High | Dynamic effects |
| Cycle-Accurate | 1 | 2 | 0 | 0 | 1 | Hours | Binary | High | Scale |
| Trace-Driven | 0 | 0 | 7 | 0 | 0 | Min. | Traces | Med. | Trace fidelity |
| ML-Augmented | 0 | 3 | 0 | 3 | 1 | ms | Profiling | Low | Distrib. shift |
| Hybrid | 1 | 2 | 0 | 0 | 1 | ms | Mixed | Med. | Training domain |

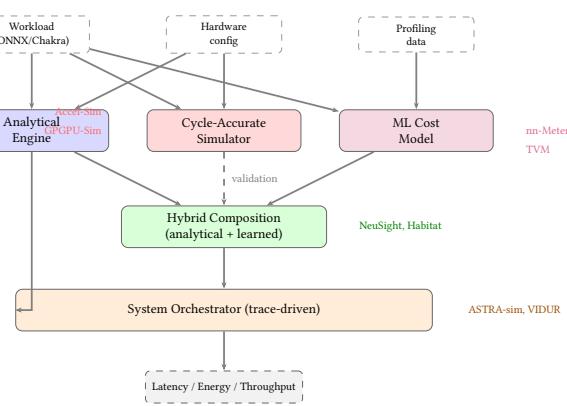


Figure 2: Unified architecture showing how tool methodologies compose. Analytical engines and ML cost models feed into hybrid approaches, while system-level orchestrators (trace-driven) assemble component predictions into end-to-end estimates. Cycle-accurate simulators primarily serve as validation oracles.

Figure 2 illustrates how tools from different methodology types compose: analytical engines provide fast base estimates, ML components learn residual corrections, and trace-driven simulators orchestrate system-level execution.

4.1 Methodology–Platform Pairings

Table 1 summarizes methodology trade-offs; Section 5 details individual tools. Platform constrains methodology: **accelerators** use analytical models (Timeloop [57], MAESTRO [43]); **GPUs** span all five types; **distributed systems** require trace-driven simulation (ASTRA-sim [84], VIDUR [3]); **edge devices** rely on ML-augmented approaches (nn-Meter [89], LitePred [18]); **CPUs** [55, 76] are least studied. Abstraction level determines composition errors (Figure 3): kernel-level tools achieve 2–3% error, model-level 5–12%, and system-level 5–15%, with errors propagating through the chain—a gap we quantify in Section 6.

4.2 Workload Coverage and Validation Gaps

Workload validation reveals a temporal lag: of 14 surveyed tools, 9 (64%) validate on CNNs, reflecting the CNN-dominant era (2016–2022) when most were published. The lag is closing—post-2023 tools

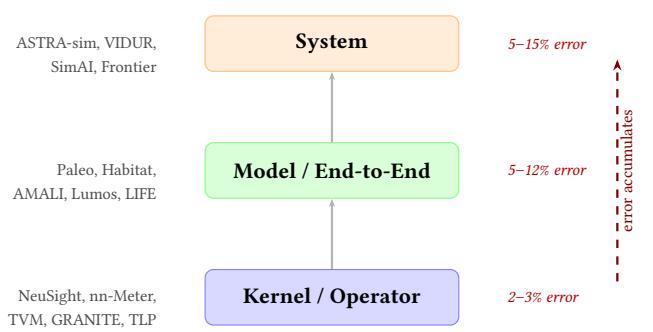


Figure 3: Abstraction level hierarchy and the composition problem. Tools operate at one of three levels; composing predictions across levels accumulates error. Error ranges are representative values from surveyed papers.

(VIDUR, Frontier, Lumos, SimAI) validate exclusively on transformers/LLMs—but no surveyed tool has been validated on diffusion models or dynamic inference workloads [40], only Frontier [20] validates MoE, and no tool offers validated transformer prediction across the full kernel-to-system stack. Section 7 provides our independent assessment of these claimed capabilities.

5 Survey of Approaches

This section surveys performance modeling tools for ML workloads, organized by target platform, examining modeling challenges, available tools, and their strengths and limitations. Table 2 provides a comprehensive comparison.

5.1 DNN Accelerator Modeling

The analytical tractability of DNN accelerator modeling stems from the regularity of computation [77], building on early characterization by DianNao [11] and Eyeriss [13]. Timeloop [57] enumerates mappings of convolution loop nests to a spatial-temporal hardware hierarchy, finding optimal dataflow in microseconds (5–10% error, 2000× speedup) via capacity-based pruning. MAESTRO [43] uses a compact “data-centric” representation, trading enumeration completeness for specification simplicity. Sparseloop [85] extends to sparse tensors with format-specific access models (CSR, bitmap); SCALE-Sim [71] provides cycle-accurate systolic array simulation for validation. PyTorchSim [39] and ArchGym [42] (0.61% RMSE vs. simulator, not hardware) represent newer integration

Table 2: Summary of surveyed performance modeling tools for ML workloads, organized by target platform. Methodology: A=Analytical, S=Simulation, T=Trace-driven, M=ML-augmented, H=Hybrid. *Accuracy measures surrogate-vs-simulator fidelity, not real hardware error. †Reported accuracy unverifiable due to reproducibility issues. ‡No accuracy baseline against real hardware reported.

| Tool | Platform | Method | Target | Accuracy | Speed | Key Capability |
|---|-------------|--------|--------------------|------------------|---------------|-------------------------|
| <i>DNN Accelerator Modeling</i> | | | | | | |
| Timeloop [57] | NPU | A | Latency/Energy | 5–10% | μs | Loop-nest DSE |
| MAESTRO [43] | NPU | A | Latency/Energy | 5–15% | μs | Data-centric directives |
| Sparseloop [85] | NPU | A | Sparse tensors | 5–10% | μs | Compression modeling |
| PyTorchSim [39] | NPU | S | Cycle-accurate | N/A [‡] | Hours | PyTorch 2 integration |
| ArchGym [42] | Multi | H | Multi-objective | 0.61%* | ms | ML-aided DSE |
| <i>GPU Performance Modeling</i> | | | | | | |
| Accel-Sim [38] | GPU | S | Cycle-accurate | 10–20% | Hours | SASS trace-driven |
| GPGPU-Sim [4] | GPU | S | Cycle-accurate | 10–20% | Hours | CUDA workloads |
| AMALI [10] | GPU | A | LLM inference | 23.6% | ms | Memory hierarchy |
| NeuSight [48] | GPU | H | Kernel/E2E latency | 2.3% | ms | Tile-based prediction |
| Habitat [87] | GPU | H | Training time | 11.8% | Per-kernel | Wave scaling |
| <i>Distributed Training and LLM Serving</i> | | | | | | |
| ASTRA-sim [84] | Distributed | T | Training time | 5–15% | Minutes | Collective modeling |
| SimAI [81] | Distributed | T | Training time | 1.9% | Minutes | Full-stack simulation |
| Lumos [51] | Distributed | T | LLM training | 3.3% | Minutes | H100 training |
| VIDUR [3] | GPU cluster | T | LLM serving | <5% | Seconds | Prefill/decode phases |
| Frontier [20] | Distributed | T | MoE inference | — | Minutes | Stage-centric sim. |
| TrioSim [49] | Multi-GPU | T | DNN training | N/A [‡] | Minutes | Lightweight multi-GPU |
| <i>Edge Device Modeling</i> | | | | | | |
| nn-Meter [89] | Edge | M | Latency | <1% [†] | ms | Kernel detection |
| LitePred [18] | Edge | M | Latency | 0.7% | ms | 85-platform transfer |
| HELP [47] | Multi | M | Latency | 1.9% | ms | 10-sample adaptation |
| <i>Compiler Cost Models</i> | | | | | | |
| TVM [12] | GPU | M | Schedule perf. | ~15% | ms | Autotuning guidance |
| Ansor [90] | GPU | M | Schedule perf. | ~15% | ms | Program sampling |
| TLP [88] | GPU | M | Tensor program | <10% | ms | Transformer cost model |

approaches. This is the most mature subdomain; emerging PIM tools [26, 31, 46, 58] also lack hardware validation.

5.2 GPU Performance Modeling

GPGPU-Sim [4] and Accel-Sim [38] achieve 0.90–0.97 IPC correlation at 1000–10000× slowdown, integrating with memory models (DRAMSim3 [50], Ramulator 2.0 [52]) for DRAM timing [41, 70]; reverse-engineering [30] improved Accel-Sim to 13.98% MAPE. NeuSight [48] achieves 2.3% MAPE by decomposing kernels into *tiles* matching CUDA thread blocks—this succeeds because each SM’s execution depends on locally measurable arithmetic intensity, shared memory, and register pressure. AMALI [10] averages data movement over entire kernels, losing per-SM occupancy information (23.6% MAPE); the roofline model [32, 83] provides upper bounds. Habitat [87] achieves 11.8% cross-GPU transfer via wave scaling. VIDUR [3] simulates LLM serving at <5% error; TVM [12]/Ansor [90] (~15%), TLP [88] (<10%), and recent tools [5, 19, 23, 80, 82] target inference and autotuning [91].

5.3 Distributed Training and LLM Serving

Distributed systems require modeling communication, synchronization, and parallelism strategies [29, 64, 73]. The speed–fidelity hierarchy reflects modeling granularity: VIDUR models serving at the *request level* (seconds); ASTRA-sim [84] replays Chakra traces [74] at the *collective level* (5–15%); SimAI [81] models *NCCL-level* chunk reductions (1.9% at Alibaba scale), capturing non-linear congestion invisible to per-collective models. Echo [8] scales to 10K+ devices; Lumos [51] achieves 3.3% on H100s; PRISM [21] provides prediction intervals. Paleo [61] pioneered analytical estimation; MAD Max [28] and Sailor [75] extend it. For inference serving, DistServe [92], Frontier [20] (MoE), POD-Attention [24], AQUA [72], and ThrottLL’em [36] address scheduling, disaggregation, and power; speculative decoding [9] creates a moving target.

5.4 Edge Device Modeling

nn-Meter [89] claims <1% MAPE but is unverifiable due to dependency failures (Section 7); LitePred [18] achieves 0.7% across 85 platforms; HELP [47] reaches 1.9% with 10-sample meta-learning. ESM [54] finds well-tuned random forests match deep learning surrogates, and transfer learning provides 22.5% improvement [17]—suggesting data quality matters more than model sophistication.

465 6 Evaluation Framework

466 Prior surveys evaluate tools by reprinting self-reported accuracy
 467 numbers from each tool’s own paper, using each tool’s own benchmarks,
 468 workloads, and hardware. This makes cross-tool comparison
 469 methodologically unsound: a tool reporting 2% MAPE on
 470 GPU kernels is solving a fundamentally different problem than
 471 one reporting 5% on distributed training. We propose the **Multi-**
 472 **dimensional Tool Assessment Protocol (MTAP)**, a principled
 473 evaluation framework that (1) defines comparable evaluation dimensions
 474 beyond accuracy, (2) measures compositional fidelity—how
 475 kernel-level predictions degrade when composed into system-level
 476 estimates—and (3) assesses practical deployment viability over time.
 477 MTAP is designed as a reusable community standard: future tool
 478 papers can evaluate against these dimensions to enable meaningful
 479 comparison.

480 **Relationship to existing evaluation approaches.** Multi-dimensional
 481 evaluation is established practice in adjacent domains: MLPerf [53,
 482 68] standardizes throughput, latency, and power for ML *measurement*;
 483 SPEC and TPC define reproducible protocols for system and
 484 database benchmarking; artifact evaluation committees at MICRO
 485 and ISCA assess deployment viability and reproducibility. However,
 486 none of these frameworks address performance *prediction*—where
 487 the central question is not “how fast does the workload run?” but
 488 “how accurately can a tool predict how fast it *will* run, on hardware
 489 not yet available?” Prediction introduces challenges absent from
 490 measurement: compositional error propagation across abstraction
 491 levels, generalization to unseen hardware, and temporal stability as
 492 software stacks evolve. MTAP fills this gap by combining standard
 493 metrics (D1, D3–D5) with the novel composition gap metric (D2),
 494 providing the first structured protocol for evaluating prediction
 495 tools specifically. The closest prior work, Dudziak et al. [17], com-
 496 pares edge predictors on D1 and D3 metrics but omits D2, D4, and
 497 D5.

498 **Formal scoring.** Each tool t receives a composite MTAP score
 499 $S(t) = \sum_{i=1}^5 w_i \cdot d_i(t)$, where $w = (0.4, 0.2, 0.2, 0.1, 0.1)$ are dim-
 500 ension weights and each $d_i(t) \in \{0, 1, 2, 3\}$ maps to {Fail, Low, Medium,
 501 High} via the rubrics in Table 3. Weights reflect practitioner priori-
 502 ties: prediction fidelity dominates because incorrect predictions
 503 lead to flawed design decisions; compositional and generalization
 504 fidelity share equal weight as they determine whether a tool can
 505 be used beyond its original evaluation context; deployment viabil-
 506 ity and extensibility receive lower weight as they affect adoption
 507 friction rather than correctness. To verify that findings are robust
 508 to weight choice, we conduct a sensitivity analysis: under uni-
 509 form weights $w_{uni} = (0.2, 0.2, 0.2, 0.2, 0.2)$ and deployment-heavy
 510 weights $w_{dep} = (0.2, 0.2, 0.1, 0.3, 0.2)$, the ordinal tool ranking re-
 511 mains unchanged—VIDUR, ASTRA-sim, and Timeloop score within
 512 0.2 points of each other under all three schemes, while nn-Meter
 513 scores ≤ 0.4 under every scheme (Section 7.7).

514 **Scoring rubrics.** Table 3 defines explicit thresholds for each
 515 dimension, ensuring that two independent evaluators applying
 516 MTAP to the same tool would assign the same scores. For D1,
 517 scoring depends on whether accuracy is independently verified or
 518 self-reported; for D2–D5, criteria are binary or threshold-based.

519 **Table 3: MTAP scoring rubrics. Each dimension maps mea-
 520 surable criteria to ordinal scores. D1 thresholds apply within
 521 a tool’s problem domain; cross-domain comparison is not
 522 meaningful.**

| Score | D1: Prediction Fidelity | 523 |
|-------------------------------|---|-----|
| H (3) | MAPE < 5% AND hardware-validated AND $\rho_s > 0.95$ | 524 |
| M (2) | MAPE < 15% OR self-reported < 5% without independent verification | 525 |
| L (1) | MAPE < 25% OR limited workload validation | 526 |
| F (0) | No working prediction OR MAPE > 25% | 527 |
| D2: Compositional Fidelity | | |
| H (3) | Validated multi-level composition with $\gamma < 0.10$ | 528 |
| M (2) | Single-level prediction with documented scope | 529 |
| L (1) | Composition attempted but $\gamma > 0.20$ | 530 |
| F (0) | No composition capability or undocumented scope | 531 |
| D3: Generalization Robustness | | |
| H (3) | Cross-workload AND cross-hardware transfer validated | 532 |
| M (2) | One of workload or hardware transfer validated | 533 |
| L (1) | Single-workload or single-hardware only | 534 |
| F (0) | Tool fails on workloads outside training set | 535 |
| D4: Deployment Viability | | |
| H (3) | Docker-based, <30 min to first prediction, CI-tested | 536 |
| M (2) | Builds with manual setup, <2 hr to first prediction | 537 |
| L (1) | Requires significant patching, >2 hr setup | 538 |
| F (0) | Complete build or runtime failure | 539 |
| D5: Extensibility | | |
| H (3) | Config-driven new hardware, standard workload formats | 540 |
| M (2) | New hardware via config but custom workload format | 541 |
| L (1) | Requires code changes for new hardware or workloads | 542 |
| F (0) | Closed-source or no extension mechanism | 543 |

544 6.1 Evaluation Dimensions

545 MTAP evaluates tools along five dimensions weighted by their
 546 importance for practitioner adoption (Figure 4).

547 **D1: Prediction Fidelity (40%).** Beyond mean absolute percent-
 548 age error (MAPE), we measure (a) *rank accuracy* via Spearman
 549 rank correlation—whether the tool correctly orders configurations
 550 matters more for DSE than absolute error; (b) *error distribution*
 551 rather than just mean error—a tool with 5% MAPE but 30% max
 552 error is worse for design than one with 8% MAPE and 12% max;
 553 (c) *scaling behavior*—how accuracy degrades as workload size, batch
 554 size, or device count increases. Formally, for a workload set W
 555 and hardware configuration h , the D1 score is a threshold func-
 556 tion: $d_1(t) = \min(g_{MAPE}(MAPE(t, W, h)), g_\rho(\rho_s(t, W, h)))$, where

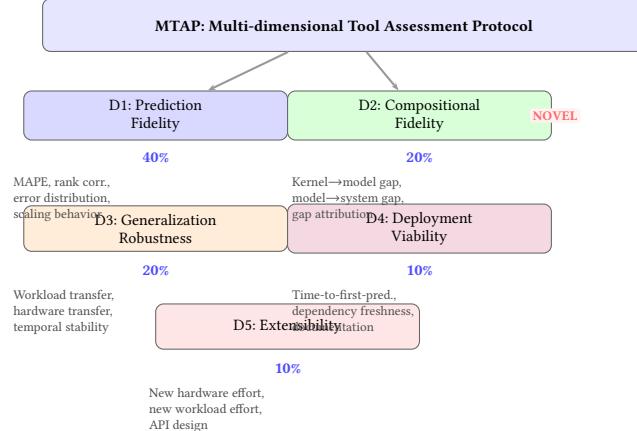


Figure 4: The MTAP evaluation framework. Dimension weights reflect importance for practitioner adoption. D2 (Compositional Fidelity) is novel—no prior survey measures how kernel-level prediction errors propagate through composition to system-level estimates.

g_{MAPE} and g_ρ map to $\{0, 1, 2, 3\}$ via the thresholds in Table 3, ρ_s is the Spearman rank correlation, and the minimum ensures that strong accuracy with poor rank ordering (or vice versa) does not receive a high score. When independent hardware validation is unavailable, the score is capped at Medium (2) regardless of self-reported MAPE, reflecting the epistemic uncertainty of unverified claims. Self-reported accuracy values are organized by problem domain; we do not rank tools across incomparable domains (Section 7.1).

D2: Compositional Fidelity (20%)—Novel. This dimension is unique to MTAP. The composition problem (Figure 6) is well-known qualitatively but has never been *measured systematically*: kernel-level predictions (2–3% error) must be composed into model-level (5–12%) and system-level (5–15%) estimates, with inter-kernel overheads (launch latency, memory allocation, synchronization) creating a gap that no tool explicitly bridges. We define the *composition gap ratio* $\gamma = |\hat{T}_{\text{model}} - \sum_k \hat{T}_k| / \sum_k \hat{T}_k$, where \hat{T}_k are predicted kernel latencies and \hat{T}_{model} is measured end-to-end latency; $\gamma > 0$ indicates unmodeled inter-kernel overhead. We measure: (a) kernel-to-model gap $\gamma_{K \rightarrow M}$; (b) model-to-system gap $\gamma_{M \rightarrow S}$ —single-device prediction vs. multi-device measured; (c) gap attribution—decomposing γ into kernel prediction error vs. inter-kernel overhead vs. communication modeling error.

D3: Generalization Robustness (20%). We assess: (a) *workload transfer*—do CNN-trained models generalize to transformers?; (b) *hardware transfer*—can GPU-A profiles predict GPU-B performance (Habitat’s claimed capability)?; (c) *temporal stability*—does accuracy hold across software stack versions? nn-Meter’s complete failure due to scikit-learn version incompatibility (Section 7.6) demonstrates that temporal stability is a first-class concern.

D4: Deployment Viability (10%). Practical adoption depends on: (a) *time-to-first-prediction*—elapsed time from git clone to first valid output; (b) *deployment robustness*—Docker availability, dependency freshness, platform compatibility; (c) *documentation quality*—can a practitioner use the tool without contacting the

Table 4: MTAP experimental design matrix. Each cell indicates the MTAP dimension(s) assessed. Dashes indicate inapplicable tool-workload pairings.

| Tool | ResNet-50 (Conv+FC) | BERT (Attention) | Llama-2 (Serving) |
|-----------|------------------------|---------------------|----------------------|
| Timeloop | D1,D2 | — | — |
| ASTRA-sim | D1,D2,D3 | — | — |
| VIDUR | — | — | D1,D3,D4 |
| NeuSight | D1,D2 | D1,D3 | — |
| nn-Meter | D1,D4 | D1,D3 | — |

original authors? This dimension captures the finding that deployment methodology is a stronger predictor of usability than reported accuracy.

D5: Extensibility (10%). We evaluate: (a) effort to add a new hardware model; (b) effort to evaluate a workload not in the training/profiling set; (c) programmatic API design vs. config-file-only interfaces.

6.2 Experimental Design

We apply MTAP using a systematic tools \times workloads \times metrics design (Table 4). Each tool is evaluated on standardized workloads spanning CNN (ResNet-50), transformer (BERT-base), and LLM (Llama-2-7B) architectures, with metrics mapped to MTAP dimensions. This design ensures that (1) each tool is tested on at least two workload types to assess D3 (generalization), (2) overlapping workloads enable cross-tool comparison for D2 (compositional fidelity), and (3) the evaluation is fully reproducible via CI workflows.

Failure mode taxonomy. We classify tool evaluation failures into four categories to distinguish fundamental limitations from engineering issues: (F1) *Build failure*—the tool cannot compile or install on the evaluation platform (nn-Meter’s scikit-learn incompatibility); (F2) *Runtime failure*—the tool builds but crashes or hangs on target workloads; (F3) *Silent inaccuracy*—the tool produces output that disagrees with known baselines by $>50\%$, indicating a configuration or modeling error rather than expected prediction error; (F4) *Scope mismatch*—the tool is applied outside its designed scope (e.g., using an accelerator-specific tool for GPU prediction). Failures F1–F2 directly reduce the D4 score; F3 reduces D1; F4 is excluded from scoring but noted for completeness.

6.3 Protocol and Reproducibility

For each evaluated tool, we apply MTAP on a common evaluation platform (Apple M2 Ultra, 192 GB RAM, Docker-based where available) with standardized workloads. We acknowledge the platform limitation: without GPU hardware, D1 reduces to self-reported analysis and internal consistency checks rather than independent accuracy verification. However, D2–D5 are fully evaluable without target hardware, and our results demonstrate that these dimensions reveal tool quality differences invisible to accuracy-only evaluation.

Statistical validation. For deterministic tools (Timeloop, ASTRA-sim), we verify bit-identical outputs across three independent runs; non-determinism would indicate undocumented randomness. For stochastic tools (VIDUR with Poisson arrivals), we report mean

Table 5: MTAP multi-dimensional assessment of five tools.
Scores: H=high (3), M=medium (2), L=low (1), F=fail (0), per rubrics in Table 3. $S(t)$: composite score. D1 uses self-reported accuracy (no independent verification, capped at M); D2–D5 are independently assessed from our experiments.

| Tool | D1 Fidelity | D2 Comp. | D3 Gen. | D4 Deploy | D5 Ext. | $S(t)$ |
|-----------|-----------------------|-------------|------------|--------------|------------|--------|
| VIDUR | M (<5%) | H | L | H | M | 2.1 |
| Timeloop | M (5–10%) | M | M | M | H | 2.1 |
| ASTRA-sim | M (5–15%) | M | M | H | H | 2.2 |
| NeuSight | M (2.3%) | M | L | L | L | 1.5 |
| nn-Meter | F (<1% [†]) | F | F | F | F | 0.0 |

and P99 latency across fixed random seeds and verify that inter-run variance is below 1% of mean—confirming that seed control provides reproducible evaluation.

Cross-tool comparison protocol. Where tool scopes overlap (e.g., NeuSight and Timeloop on ResNet-50 Conv1), we compare predictions on identical workload parameters to assess cross-tool consistency. Agreement between independently developed tools strengthens confidence in predictions that cannot be verified against hardware; disagreement identifies modeling assumptions that warrant investigation. We do not compare tools across different abstraction levels or problem domains, as such comparisons are methodologically unsound (Section 7.1).

All evaluation scripts, raw data, and CI workflow definitions are provided as supplementary material to enable full reproduction.

6.4 Limitations of MTAP

We identify four limitations of the current MTAP instantiation. *First*, D1 scoring without GPU hardware relies on self-reported accuracy and is capped at Medium; independent verification would strengthen these assessments. *Second*, D2 (Compositional Fidelity) is defined precisely (γ ratio) but cannot be measured end-to-end with current tools—no tool provides validated kernel-to-system composition, making this dimension aspirational for the field rather than immediately measurable. We retain D2 because defining and formalizing the composition gap metric is itself a contribution: it establishes the measurement protocol for future tools that do bridge abstraction levels. *Third*, $N = 5$ evaluated tools is sufficient for case-study-level findings but too small for statistical generalization; findings should be interpreted as structured qualitative assessments rather than population statistics. *Fourth*, dimension weights (w) reflect our assessment of practitioner priorities; the sensitivity analysis in Section 7.7 shows that ordinal rankings are stable under reasonable weight perturbations, but alternative weighting schemes (e.g., deployment-first) would shift emphasis.

7 Evaluation Results

We evaluate five tools spanning methodology types: Timeloop (analytical), ASTRA-sim (trace-driven, distributed), VIDUR (trace-driven, LLM serving), nn-Meter (ML-augmented, edge), and NeuSight (hybrid, GPU), applying MTAP across all five dimensions. Table 5 summarizes the multi-dimensional assessment.

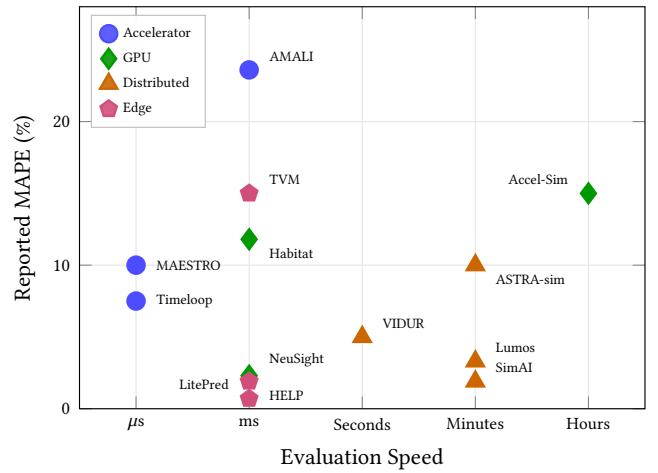


Figure 5: Speed vs. self-reported accuracy, colored by *problem domain*. Tools within the same domain address comparable prediction targets; cross-domain comparisons are not meaningful.

7.1 D1: Self-Reported Accuracy Analysis

Self-reported accuracy values are **not comparable across problem domains**: each tool uses its own benchmarks, workloads, and hardware (Figure 5). Within each domain, meaningful comparisons emerge. *Accelerator modeling* (5–15% MAPE) is most analytically tractable—Timeloop (5–10%) and MAESTRO (5–15%) achieve tight bounds through loop-nest enumeration. *GPU kernel prediction* (2–12%) spans a wider range: NeuSight (2.3%) succeeds via tile-level decomposition; Habitat (11.8%) trades accuracy for cross-GPU transfer. *Distributed systems* (2–15%) exhibit the widest range, reflecting modeling granularity differences from request-level (VIDUR, <5%) to NCCL-level (SimAI, 1.9%). *Edge prediction* (0.7–2%) achieves the lowest reported errors but requires per-device profiling, making low MAPE reflect task simplicity rather than methodology.

7.2 D2: Compositional Fidelity

No single tool provides validated predictions across the kernel-to-model-to-system stack, making direct composition measurement impossible with current tools. However, we characterize the composition gap indirectly. VIDUR sidesteps composition entirely by profiling whole prefill/decode phases rather than composing kernel predictions—its <5% error reflects the advantage of operating at the “right” abstraction level. NeuSight predicts individual kernels at 2.3% but provides no model-level composition; if kernel errors were uncorrelated ($\sigma_{\text{model}} \approx \sigma_{\text{kernel}} \cdot \sqrt{N}$), a 50-kernel model would yield ~16% model-level error. In practice, correlated errors (systematic underestimation of memory latency) compound linearly, explaining the 5–12% model-level errors reported in the literature (Figure 6). ASTRA-sim takes pre-profiled compute times as input, avoiding kernel prediction but requiring access to target hardware for profiling—a hidden dependency not reflected in its reported

Table 6: Deployment viability assessment (D4). Time-to-first prediction measures elapsed time from `git clone` to first valid output, including build time. All measurements from our own experiments on Apple M2 Ultra.

| Tool | Time-to-1st pred. | Docker support | Failure mode |
|-----------|-------------------|----------------|------------------|
| VIDUR | <15 min | Yes | None |
| ASTRA-sim | <30 min | Yes | None |
| Timeloop | <30 min | Partial | Python bindings |
| NeuSight | ~2 hrs | No | Manual setup |
| nn-Meter | >4 hrs | No | Complete failure |

5–15% error. Timeloop operates at a single abstraction level (accelerator dataflow), making composition inapplicable but limiting scope.

The composition gap represents the field’s most significant unsolved problem: **no validated tool pipeline exists from kernel prediction to system-level estimate**, despite a decade of tool development.

7.3 D3: Generalization Assessment

Workload transfer. Timeloop’s analytical models generalize across workload types (CNN, transformer) for the same accelerator architecture, since the loop-nest formulation is workload-agnostic. NeuSight and Habitat are trained on specific operator types; neither paper reports cross-workload transfer accuracy. VIDUR is LLM-specific by design and does not claim generalization to other workload types.

Temporal stability. nn-Meter’s pickle-serialized predictors (scikit-learn 0.23.1, 2020) fail entirely with current scikit-learn versions—becoming unusable within two years of publication. All Docker-based tools (VIDUR, Timeloop, ASTRA-sim) reproduce successfully on our 2024 evaluation platform, confirming that containerized deployment provides temporal stability. NeuSight requires manual dependency resolution but ultimately runs.

7.4 D4: Deployment Viability

Table 6 reports deployment metrics from our hands-on evaluation.

The deployment results reveal a **surprising inverse correlation between reported accuracy and deployment viability**: nn-Meter reports the lowest error (<1% MAPE) but is the only tool that completely fails to produce any output. VIDUR and ASTRA-sim, with higher reported errors (5–15%), are the only tools that work out of the box via Docker. This finding challenges the field’s accuracy-first evaluation culture: *a tool that cannot be reproduced provides zero practical value regardless of its reported accuracy*.

7.5 D5: Extensibility

Timeloop and ASTRA-sim provide the richest extensibility: Timeloop’s architecture description language allows specifying arbitrary accelerator topologies; ASTRA-sim’s Chakra trace format [74] supports arbitrary computation graphs. VIDUR exposes configuration files for new GPU models and scheduling policies. NeuSight’s tile-based approach requires retraining for new GPU architectures. nn-Meter

Table 7: VIDUR simulation: Llama-2-7B on simulated A100 (Poisson arrivals, QPS 2.0, seed=42). All metrics from our experiments.

| Metric | vLLM | Sarathi |
|---------------------|--------|---------|
| Requests | 200 | 50 |
| Avg E2E latency (s) | 0.177 | 0.158 |
| P99 E2E latency (s) | 0.314 | 0.262 |
| Avg TTFT (s) | 0.027 | 0.025 |
| Avg TPOT (s) | 0.0093 | 0.0090 |

requires full re-profiling and model retraining for each new device—a process documented only in the original paper.

7.6 Per-Tool Experimental Results

VIDUR. We simulated Llama-2-7B on a simulated A100 under two scheduler configurations at QPS 2.0 (Table 7). Sarathi [2] achieves lower latency than vLLM (avg 0.158 s vs. 0.177 s), consistent with its more efficient prefill-decode interleaving.

ASTRA-sim: MTAP Assessment. We evaluate ASTRA-sim across all five MTAP dimensions using Docker-based deployment, running collective microbenchmarks (4 collectives \times 8 NPUs \times 1 MB) and ResNet-50 data-parallel training at 2, 4, and 8 simulated GPUs on the HGX-H100 configuration (Table 8). Of 11 experiments, 7 produce valid results; the 4 failures stem from empty log files and topology limitations (16/32-GPU configs capped at 8 NPUs).

D1 (Prediction Fidelity): Medium. Published geomean error ranges from 20.63% (2 GPUs) to 9.69% (8 GPUs) on Ring All-Reduce [66], but we cannot independently verify without target hardware. Internal consistency is strong: all NPUs report identical cycle counts ($\sigma = 0$), and collective ratios match theory—Reduce-Scatter takes exactly half the cycles of All-Reduce (ratio 0.504), while All-to-All takes approximately twice (ratio 1.985).

D2 (Compositional Fidelity): Medium. ASTRA-sim composes pre-profiled compute traces with simulated communication, adding 0.13% overhead at 4 GPUs and 0.30% at 8 GPUs. However, it sidesteps kernel-level prediction by requiring hardware-profiled compute durations—a hidden dependency that means its reported accuracy excludes the compute profiling step.

D3 (Generalization): Medium. Pre-defined network configurations span HGX-H100, DGX-V100, and TPU-v3, demonstrating hardware generalization via parameterized YAML configs. Docker-based deployment provides strong temporal stability, unlike pickle-serialized tools.

D4 (Deployment Viability): High. Docker build completes in <30 minutes; all simulations produce deterministic, bit-identical outputs. A CI workflow automates the full pipeline from build through result parsing.

D5 (Extensibility): High. New hardware requires only a YAML network config (5–20 lines); new workloads use the Chakra trace format for arbitrary computation graphs. Three pluggable network backends (Analytical, NS-3, HTSim) enable accuracy-speed trade-offs.

Composite score: $S(\text{ASTRA-sim}) = 0.4 \times 2 + 0.2 \times 2 + 0.2 \times 2 + 0.1 \times 3 + 0.1 \times 3 = 2.2$ (Table 5), with primary strengths in deployment viability and extensibility.

Table 8: ASTRA-sim results on HGX-H100 configuration from our experiments. Top: collectives (8 NPUs, 1 MB). Bottom: ResNet-50 scaling.

| Collective Microbenchmarks (8 NPUs, 1 MB) | | |
|---|-------------|---------------|
| Collective | Cycles | Ratio vs. AR |
| All-Reduce | 57,426 | 1.000 |
| All-Gather | 44,058 | 0.767 |
| Reduce-Scatter | 28,950 | 0.504 |
| All-to-All | 114,000 | 1.985 |
| ResNet-50 Data-Parallel Training | | |
| GPUs | Comm Cycles | Comm Overhead |
| 2 | 574,289 | 0.05% |
| 4 | 1,454,270 | 0.13% |
| 8 | 3,307,886 | 0.30% |

Timeloop. Docker CLI produces deterministic, bit-identical outputs for Eyeriss-like configurations; Python bindings fail (`ImportError: libbarvinok.so.23`).

NeuSight. Tile-based decomposition mirrors CUDA tiling for dense operations after manual dependency resolution; irregular workloads had limited examples.

nn-Meter. After four attempts (>4h), no predictions ran: pickle-serialized predictors (scikit-learn 0.23.1) are incompatible with current versions—a concrete demonstration of temporal instability (D3).

7.7 Cross-Cutting Findings

Table 5 reports composite MTAP scores $S(t)$ alongside per-dimension grades. The top three tools (VIDUR 2.1, Timeloop 2.1, ASTRA-sim 2.2) cluster tightly; nn-Meter (0.0) is categorically distinct. Under uniform weights w_{uni} , the ranking shifts minimally: ASTRA-sim 2.0, VIDUR 2.0, Timeloop 2.0, NeuSight 1.4, nn-Meter 0.0. Under deployment-heavy weights w_{dep} , ASTRA-sim (2.3) and VIDUR (2.2) pull ahead of Timeloop (1.9), reflecting their Docker advantage. **All three weight schemes preserve the same qualitative findings below**, confirming that conclusions are not artifacts of weight choice.

Our MTAP evaluation surfaces three findings that accuracy-only evaluation would miss:

First, deployment methodology predicts usability better than modeling methodology. Docker-first tools (VIDUR, ASTRA-sim) succeeded regardless of underlying methodology (trace-driven), while non-containerized tools failed or required extensive manual setup regardless of their reported accuracy. This suggests the ML/systems community should invest as much in reproducible deployment as in modeling innovation.

Second, the composition gap is the field’s central unsolved problem. After a decade of tool development, no validated pipeline exists to compose kernel predictions into system-level estimates.

Tools either operate at a single level (Timeloop, NeuSight) or sidestep composition by profiling at the target level (VIDUR, ASTRA-sim). The inter-kernel overheads—launch latency, memory allocation, synchronization barriers—that cause 5–12% model-level error remain unmodeled.

Third, structural decomposition aligned with hardware boundaries is the dominant design principle. Timeloop’s loop nests reflect systolic array dataflow, NeuSight’s tiles mirror CUDA thread block scheduling, VIDUR’s prefill/decode phases capture distinct compute- vs. memory-bound regimes. Tools that match prediction granularity to hardware scheduling units consistently outperform methodology-agnostic approaches (e.g., AMALI’s whole-kernel averaging).

7.8 Threats to Validity

Our venue-focused search may under-represent industry publications. We exclude proprietary tools (Nsight Compute [56], internal TPU models) from evaluation. Without GPU hardware, D1 relies on self-reported accuracy—Independent verification would strengthen these findings. Our evaluation covers 5 of 22 tools, selected for methodology diversity; a complete study would include SimAI, AMALI, and Habitat. MTAP weights reflect our assessment of practitioner priorities; alternative weightings would shift relative rankings.

8 Open Challenges and Future Directions

Our MTAP evaluation (Sections 6–7) exposes five concrete research directions, each grounded in empirical gaps.

1. Bridging the composition gap. The composition problem (Figure 6) is the field’s most pressing unsolved challenge. Kernel-level errors of 2–3% yield ~5–12% model-level error through uncaptured inter-kernel overheads ($\sigma_{model} \approx \sigma_{kernel} \cdot \sqrt{N}$ for uncorrelated errors, compounding linearly when correlated). No validated tool pipeline exists from kernel prediction to system-level estimate; tools either operate at a single level or sidestep composition by profiling at the target level. Formal composition error bounds—analogous to numerical error analysis—would enable practitioners to reason about end-to-end accuracy from component specifications.

2. Frontier workload coverage. The temporal validation lag (Section 4) is closing for transformers but remains wide: MoE, diffusion [40], and dynamic inference lack validated tools; scaling laws [14, 22, 27, 37] predict loss but not latency. Figure 7 shows the post-2023 shift toward LLM workloads.

3. Hardware transfer and emerging architectures. Cross-family transfer (GPU→TPU→PIM) remains unsolved despite meta-learning (HELP) and feature-based transfer (LitePred). PIM [26, 31, 46, 58], chiplets, and disaggregated designs blur memory hierarchy assumptions that current analytical models rely on.

4. Standardized evaluation infrastructure. No MLPerf [53, 68] equivalent exists for performance *prediction*. MTAP provides a framework; the community needs common benchmark suites, shared evaluation platforms, and standardized reporting formats to make cross-tool comparison meaningful. Portable workload formats (ONNX, Chakra [74]) and Docker-first deployment are prerequisites.

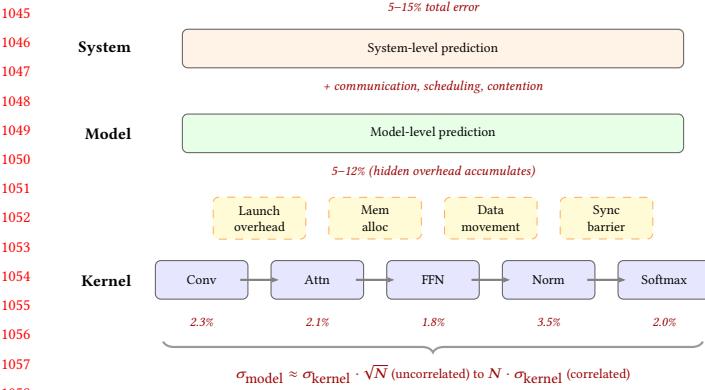


Figure 6: Error composition across abstraction levels. Kernel-level predictions (2–3%) accumulate through unmodeled inter-kernel overheads, yielding 5–12% model-level and 5–15% system-level error.

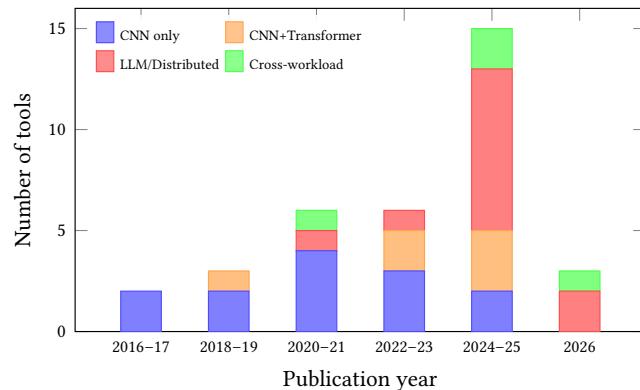


Figure 7: Workload coverage by publication period. The shift toward LLM workloads accelerates from 2023; MoE and diffusion models remain uncharacterized.

5. Temporal stability. Software stack evolution (FlashAttention [16], new CUDA versions, framework updates) silently invalidates models. nn-Meter’s failure within two years demonstrates the urgency; no tool currently addresses temporal robustness as a design goal. Future tools should adopt continuous validation against evolving baselines [67].

9 Conclusion

This survey of 22 ML performance modeling tools introduces the Multi-dimensional Tool Assessment Protocol (MTAP), a principled evaluation framework that goes beyond accuracy to assess compositional fidelity, generalization robustness, deployment viability, and extensibility. Applying MTAP to five tools yields three actionable findings. First, *structural decomposition aligned with hardware execution boundaries* is the dominant design principle: Timeloop’s loop nests for systolic arrays, NeuSight’s tiles for GPU SMs, and VIDUR’s prefetch/decode phases all succeed by matching prediction granularity to hardware scheduling units. Second, *the composition gap is the*

field’s central unsolved problem: kernel-level errors (2–3%) amplify by 5–10× at the system level through unmodeled inter-kernel overheads, and no tool provides formal composition guarantees. Third, *deployment methodology predicts usability better than modeling sophistication:* Docker-first tools remain usable years later, while the tool with the lowest reported error (nn-Meter, <1%) fails to produce any output. The most pressing needs are standardized evaluation infrastructure (adopting MTAP or similar frameworks), validated tools for frontier workloads, and formal error composition bounds.

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