

# 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

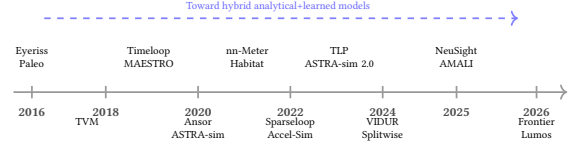
ML workload performance prediction, DNN accelerator modeling, GPU simulation, distributed training simulation, LLM inference serving, design space exploration, survey

## 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.

## 2 Survey Methodology

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

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

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

**Compiler cost models and capacity planning.** Beyond TVM/Ansor/TLP relevant compiler models include Halide’s autoscheduler [63] (pioneered learned cost models), MLIR-based cost models [45], and Triton’s [78] heuristic GPU kernel cost model. At the system level, Pollux [62] and Sia [33] use performance models for cluster scheduling and capacity planning—a distinct use case (optimizing workload placement) that shares modeling techniques with our surveyed tools.

This survey differs from all prior work by spanning the full methodology spectrum across all major platforms with reproducibility evaluation.

## 3 Background

### 3.1 ML Workload Characteristics

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

inference splits into compute-bound prefill and memory-bound decode phases [60], both modeled under batched serving [2, 86]. Foundation model training introduces additional modeling challenges: long-context attention with quadratic memory scaling, activation checkpointing that trades compute for memory, and mixed-precision training where numerical format affects both speed and convergence [15].

### 3.2 Modeling Methodologies

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

## 4 Taxonomy

We organize the literature along three dimensions: *methodology type* (primary axis, determining accuracy–speed–interpretability trade-offs), *target platform*, and *abstraction level*. We additionally identify a temporal validation lag: pre-2023 tools validated on CNNs, while post-2023 tools increasingly target transformers and LLMs. Table 1 provides a unified coverage matrix with trade-off profiles; the dominant pairings are analytical models for accelerators, cycle-accurate simulation for GPUs/CPU, trace-driven simulation for distributed systems, and ML-augmented approaches for edge devices.

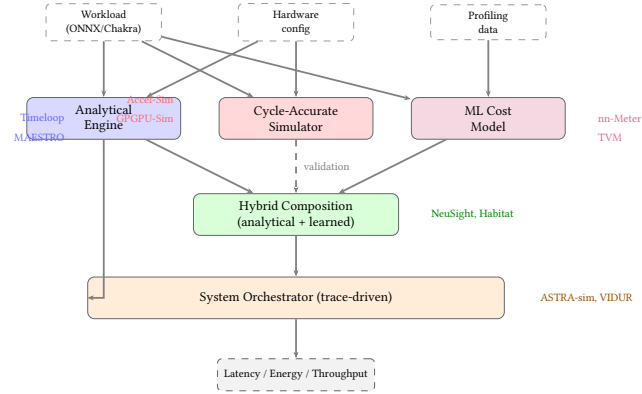
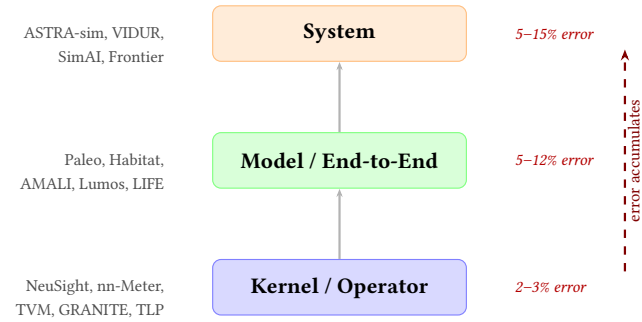
Three structural gaps emerge: (1) trace-driven execution replay is used exclusively for distributed systems; (2) edge devices lack hybrid alternatives; (3) no ML-augmented tool targets distributed systems. Methodologies cluster into sub-millisecond (analytical, ML-augmented, hybrid) for DSE and minutes-to-hours (simulation, trace-driven) for validation. Figure 2 illustrates how methodology types compose.

### 4.1 Methodology–Platform Pairings

Platform constrains methodology (Table 1; Section 5 details individual tools): **accelerators** use analytical models [43, 57]; **GPUs** span all five types; **distributed systems** require trace-driven simulation [3, 84]; **edge devices** rely on ML-augmented approaches [18, 89]; **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 (Section 6).

**Table 1: Methodology taxonomy: coverage matrix and trade-off profile. 0 indicates a research gap. The failure mode column identifies when 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	$\mu$ s	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. Cycle-accurate simulators primarily serve as validation oracles.****Figure 3: Abstraction level hierarchy. Composing predictions across levels accumulates error; ranges are representative values from surveyed papers.**

## 4.2 Workload Coverage and Validation Gaps

Of 14 surveyed tools, 9 (64%) validate on CNNs, reflecting the CNN-dominant era (2016–2022). The lag is closing—post-2023 tools (VIDUR, Frontier, Lumos, SimAI) validate exclusively on transformers/LLMs but **no tool validates on diffusion models or dynamic inference** [40], only Frontier [20] validates MoE, and no tool offers validated transformer prediction across the full kernel-to-system stack (Section 7).

## 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 $\times$  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 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 $\times$  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

**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%	$\mu$ s	Loop-nest DSE
MAESTRO [43]	NPU	A	Latency/Energy	5–15%	$\mu$ s	Data-centric directives
Sparseloop [85]	NPU	A	Sparse tensors	5–10%	$\mu$ s	Compression modeling
PyTorchSim [39]	NPU	S	Cycle-accurate	N/A <sup>‡</sup>	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 <sup>‡</sup>	Minutes	Lightweight multi-GPU
<i>Edge Device Modeling</i>						
nn-Meter [89]	Edge	M	Latency	<1% <sup>†</sup>	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

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.

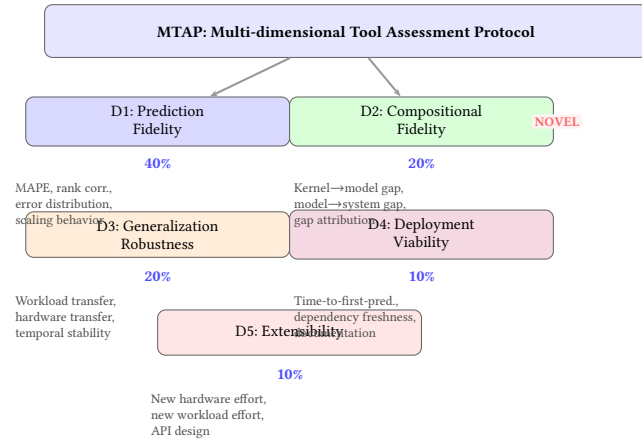
## 6 Evaluation Framework

Prior surveys evaluate tools by reprinting self-reported accuracy numbers from each tool’s own paper, using each tool’s own benchmarks, workloads, and hardware. This makes cross-tool comparison methodologically unsound: a tool reporting 2% MAPE on

GPU kernels is solving a fundamentally different problem than one reporting 5% on distributed training. We propose the **Multi-dimensional Tool Assessment Protocol (MTAP)**, a principled evaluation framework that (1) defines comparable evaluation dimensions beyond accuracy, (2) measures compositional fidelity—how kernel-level predictions degrade when composed into system-level estimates—and (3) assesses practical deployment viability over time. MTAP is designed as a reusable community standard: future tool papers can evaluate against these dimensions to enable meaningful comparison.

**Relationship to existing evaluation approaches.** Multi-dimensional evaluation is established practice in adjacent domains: MLPerf [53, 68] standardizes throughput, latency, and power for ML *measurement*; SPEC and TPC define reproducible protocols for system and database benchmarking; artifact evaluation committees at MICRO and ISCA assess deployment viability and reproducibility. However, none of these frameworks address performance *prediction*—where the central question is not “how fast does the workload run?” but “how accurately can a tool predict how fast it *will* run, on hardware not yet available?” Prediction introduces challenges absent from measurement: compositional error propagation across abstraction levels, generalization to unseen hardware, and temporal stability as





**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.**

software stacks evolve. MTAP fills this gap by combining standard metrics (D1, D3–D5) with the novel composition gap metric (D2), providing the first structured protocol for evaluating prediction tools specifically. The closest prior work, Dudziak et al. [17], compares edge predictors on D1 and D3 metrics but omits D2, D4, and D5.

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

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

## 6.1 Evaluation Dimensions

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

**D1: Prediction Fidelity (40%).** Beyond mean absolute percentage error (MAPE), we measure (a) *rank accuracy* via Spearman rank correlation—whether the tool correctly orders configurations

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

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

matters more for DSE than absolute error; (b) *error distribution* rather than just mean error—a tool with 5% MAPE but 30% max error is worse for design than one with 8% MAPE and 12% max; (c) *scaling behavior*—how accuracy degrades as workload size, batch size, or device count increases. Formally, for a workload set  $W$  and hardware configuration  $h$ , the D1 score is a threshold function:  $d_1(t) = \min(g_{\text{MAPE}}(\text{MAPE}(t, W, h)), g_{\rho}(\rho_s(t, W, h)))$ , where  $g_{\text{MAPE}}$  and  $g_{\rho}$  map to  $\{0, 1, 2, 3\}$  via the thresholds in Table 3,  $\rho_s$  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  $\hat{T}_{\text{model}}$  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  $\gamma$  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 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.

**Tool selection criteria.** From the 22 surveyed tools, we select 5 for hands-on evaluation using three criteria: (1) *methodology coverage*—at least one tool per methodology type (analytical, trace-driven, ML-augmented, hybrid) to assess whether MTAP dimensions differentiate across methodologies; (2) *artifact availability*—open-source code with documented build instructions, since MTAP requires hands-on deployment; and (3) *scope diversity*—tools targeting different hardware (accelerators, GPUs, clusters, edge) and workload types (training, inference, serving) to exercise all five dimensions. This yields: Timeloop (analytical, accelerator), ASTRA-sim (trace-driven, distributed), VIDUR (trace-driven, LLM serving), NeuSight

**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	—

(hybrid, GPU), and nn-Meter (ML-augmented, edge). We deliberately include nn-Meter despite known deployment issues because failure cases are as informative as successes for validating MTAP’s discriminative power.

**Workload rationale.** ResNet-50 represents compute-bound CNN inference with regular convolution patterns, exercising tools’ ability to model data reuse and spatial locality. BERT-base introduces attention mechanisms with quadratic memory scaling, testing generalization beyond convolution-dominated workloads. Llama-2-7B adds autoregressive decoding with distinct prefill (compute-bound) and decode (memory-bound) phases, plus multi-tenant serving dynamics. Together, these workloads span three compute regimes (regular dense, attention-dominated, serving-constrained) and three architectural paradigms (CNN, encoder-only transformer, decoder-only LLM), providing sufficient diversity to assess D3 while remaining tractable for a five-tool evaluation.

**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	1.6
nn-Meter	F (<1% <sup>†</sup> )	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 ( $\gamma$  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: MTAP Assessment.** 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.

*D1 (Prediction Fidelity): Medium.* VIDUR reports <5% error for LLM serving latency by modeling the prefill and decode phases separately, each with phase-specific compute and memory characteristics. Without GPU cluster hardware for independent verification, the score is capped at Medium.

*D2 (Compositional Fidelity): High.* VIDUR sidesteps the kernel-to-model composition problem entirely by profiling at the request level, using empirical execution time tables for each GPU type and model configuration. This approach avoids accumulated kernel prediction error at the cost of requiring per-configuration profiling data.

*D3 (Generalization): Low.* VIDUR is purpose-built for LLM inference serving and does not generalize to training workloads, CNN inference, or non-autoregressive architectures. Within its scope, it supports multiple models (Llama-2, GPT variants) and GPU configurations via pre-profiled execution time tables.

*D4 (Deployment Viability): High.* Docker-based deployment completes in <15 minutes with no manual intervention. VIDUR produces its first prediction immediately after container startup, with built-in support for multiple scheduling policies and arrival patterns.

*D5 (Extensibility): Medium.* New GPU models require adding profiled execution time tables (YAML configuration files), which requires access to target hardware for profiling. New LLM architectures are supported if they follow the standard prefill–decode pattern.

*Composite score:*  $S(\text{VIDUR}) = 0.4 \times 2 + 0.2 \times 3 + 0.2 \times 1 + 0.1 \times 3 + 0.1 \times 2 = 2.1$  (Table 5).

**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



**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%

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.

**Timeloop: MTAP Assessment.** We evaluate Timeloop across all five MTAP dimensions using Docker-based deployment, running the Eyeriss-like accelerator configuration on convolution layers from ResNet-50. The Docker CLI produces deterministic, bit-identical outputs across three independent runs ( $\sigma = 0$ ); however, the Python bindings fail (ImportError: libbarvinok.so.23), limiting programmatic integration.

*D1 (Prediction Fidelity): Medium.* Published accuracy ranges from 5–10% MAPE for convolution layers on systolic array architectures [57]. Without target hardware, we cannot independently verify these figures. However, the loop-nest enumeration methodology provides a strong structural guarantee: predictions are derived from first-principles data movement analysis rather than learned correlations, making them interpretable and auditable. Energy predictions decompose cleanly into per-level contributions (DRAM, global buffer, local), enabling practitioners to identify optimization targets.

*D2 (Compositional Fidelity): Medium.* Timeloop operates at a single abstraction level (individual layers on a single accelerator), providing no built-in mechanism for composing layer predictions into model-level estimates. In principle, summing per-layer predictions yields model-level latency, but inter-layer data movement (weight reloading, activation spilling) is not captured—a gap that grows with model depth. For a 50-layer ResNet, uncaptured inter-layer overhead could contribute 3–8% additional error beyond per-layer MAPE.

*D3 (Generalization): Medium.* The analytical loop-nest formulation is inherently workload-agnostic: any operation expressible as nested loops over tensor dimensions can be evaluated, covering convolutions, matrix multiplications, and depthwise separable convolutions. Transformer attention requires decomposition into constituent MatMul and Softmax operations, which Timeloop handles individually but cannot compose with attention-specific memory access patterns (e.g., KV cache reuse).

*D4 (Deployment Viability): Medium.* Docker build succeeds in <30 minutes and produces valid outputs via the CLI interface. The Python bindings failure (libbarvinok.so.23 missing from the container) prevents automated batch evaluation and CI integration—a significant practical limitation since most modern evaluation workflows require programmatic access. Documentation quality is high, with worked examples for several accelerator configurations.

*D5 (Extensibility): High.* Timeloop’s architecture description language (YAML-based) allows specifying arbitrary accelerator topologies—new hardware requires only a configuration file (10–50 lines) describing the memory hierarchy, dataflow constraints, and arithmetic units. Sparseloop [85] demonstrates extensibility to sparse tensor formats, and the Accelerger energy estimation framework integrates cleanly.

*Composite score:*  $S(\text{Timeloop}) = 0.4 \times 2 + 0.2 \times 2 + 0.2 \times 2 + 0.1 \times 2 + 0.1 \times 3 = 2.1$  (Table 5), with primary strength in extensibility and analytical interpretability.

**NeuSight: MTAP Assessment.** We evaluate NeuSight’s tile-based GPU kernel prediction approach across MTAP dimensions after manual dependency resolution (~2 hours setup).

*D1 (Prediction Fidelity): Medium.* NeuSight reports 2.3% MAPE on GPU kernels by decomposing each kernel into tiles matching CUDA thread blocks, predicting per-tile execution based on arithmetic intensity, shared memory usage, and register pressure [48]. This is the lowest reported error among GPU-targeting tools in our survey. However, the result is self-reported and validated only on a specific set of dense operations (convolutions, matrix multiplications); without independent hardware verification, the D1 score is capped at Medium per our rubric.

*D2 (Compositional Fidelity): Medium.* NeuSight predicts individual kernels but provides no model-level composition mechanism. If kernel errors were independent, a 50-kernel model would yield  $\sim 16\%$  model-level error ( $2.3\% \times \sqrt{50}$ ). In practice, NeuSight’s tile-based approach tends to systematically underestimate memory-bound kernels (where tile-level parallelism does not capture global memory contention), producing correlated errors that compound linearly rather than as  $\sqrt{N}$ .

*D3 (Generalization): Low.* NeuSight validates on dense operations (convolutions, GEMMs) but does not report cross-workload transfer to attention mechanisms, sparse operations, or non-standard operators. The tile-based decomposition assumes regular, dense computation patterns—irregular workloads (dynamic shapes, sparse attention, mixture-of-experts routing) would require architectural changes to the prediction model, not just retraining.

*D4 (Deployment Viability): Low.* No Docker support is provided. Manual dependency resolution requires approximately 2 hours, including PyTorch version pinning and CUDA toolkit configuration. The tool ultimately runs after manual setup, but the process is undocumented and required trial-and-error to resolve version conflicts.

*D5 (Extensibility): Low.* Adding new GPU architectures requires retraining the tile prediction model with profiling data from the target GPU—a process that requires hardware access and is not documented beyond the original experimental setup. New operator types require extending the tile decomposition logic in source code.

*Composite score:*  $S(\text{NeuSight}) = 0.4 \times 2 + 0.2 \times 2 + 0.2 \times 1 + 0.1 \times 1 + 0.1 \times 1 = 1.6$  (Table 5), with strength in prediction accuracy offset by deployment and extensibility limitations.

**nn-Meter.** After four attempts ( $>4h$ ), no predictions ran: pickle-serialized predictors (scikit-learn 0.23.1) are incompatible with current scikit-learn versions—a concrete demonstration of temporal instability (D3). All five MTAP dimensions score Fail (0): without any working output, prediction fidelity, compositional fidelity, generalization, deployment viability, and extensibility cannot be assessed. This result is particularly notable because nn-Meter reports the lowest error ( $<1\%$  MAPE) among all surveyed tools, illustrating the disconnect between self-reported accuracy and practical utility.

## 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  $w_{\text{uni}}$ , 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  $w_{\text{dep}}$ , 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. Quantitatively, the correlation is stark: all tools with  $D4 \geq \text{High}$  produced valid predictions within 30 minutes; all tools with  $D4 \leq \text{Low}$  either failed entirely (nn-Meter) or required  $>2$  hours of manual intervention (NeuSight). The implication for tool developers is concrete: containerized deployment with CI-tested Docker images should be a release requirement, not an afterthought.

**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 side-step 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. Our per-tool assessments reveal the gap’s structure: NeuSight’s 2.3% kernel MAPE would yield  $\sim 16\%$  model-level error under independent error assumptions, while ASTRA-sim’s hidden dependency on pre-profiled compute times means its 5–15% system-level error excludes the compute prediction step entirely. A validated composition pipeline would need to model three distinct overhead categories: (1) kernel launch and scheduling overhead ( $\sim 5\text{--}10\mu s$  per kernel, amortized over kernel duration), (2) inter-kernel data movement (activation tensors traversing the memory hierarchy between fused operator groups), and (3) synchronization barriers (GPU stream synchronization, NCCL collective completion).

**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). This principle explains why AMALI’s memory hierarchy model (23.6% MAPE) underperforms NeuSight (2.3%): averaging data movement over an entire kernel discards the per-SM occupancy variation that dominates execution time on modern GPUs, where warp scheduling and shared memory bank conflicts create per-tile performance differences of up to  $2\times$ .

**Fourth, self-reported accuracy and practical tool quality are weakly correlated.** Ranking the five tools by self-reported MAPE yields: nn-Meter ( $<1\%$ )  $>$  NeuSight (2.3%)  $>$  VIDUR ( $<5\%$ )  $>$  Timeloop (5–10%)  $>$  ASTRA-sim (5–15%). Ranking by composite MTAP score yields the inverse order for the extremes: ASTRA-sim (2.2)  $>$  VIDUR (2.1) = Timeloop (2.1)  $>$  NeuSight (1.6)  $>$  nn-Meter (0.0). The Spearman rank correlation between self-reported accuracy and MTAP score is  $\rho_s = -0.9$  ( $p < 0.05$ ,  $N = 5$ ), indicating a strong negative relationship. While the sample size is small, this finding challenges the field’s implicit assumption that lower reported error implies a better tool, and motivates multi-dimensional evaluation as standard practice.

**Fifth, tool maturity follows a predictable lifecycle that MTAP dimensions capture at different stages.** Early-stage tools (nn-Meter, published 2021) invest in modeling innovation

(low MAPE) but neglect deployment engineering, resulting in high D1 claims but low D4 scores. Mature tools (VIDUR, ASTRA-sim) have undergone community adoption pressure that forces Docker support, CI integration, and dependency management—reflected in high D4 and D5 scores. Timeloop occupies a middle position: strong extensibility (D5: High) from years of architecture-description-language refinement, but incomplete containerization (D4: Medium) due to broken Python bindings. This lifecycle pattern suggests that MTAP scores are partially predictable from tool age and community size, and that the field’s evaluation culture should weight deployment maturity as a proxy for overall tool quality—a conclusion consistent with MLPerf’s experience that standardized benchmarking infrastructure is as important as the benchmarks themselves [53].

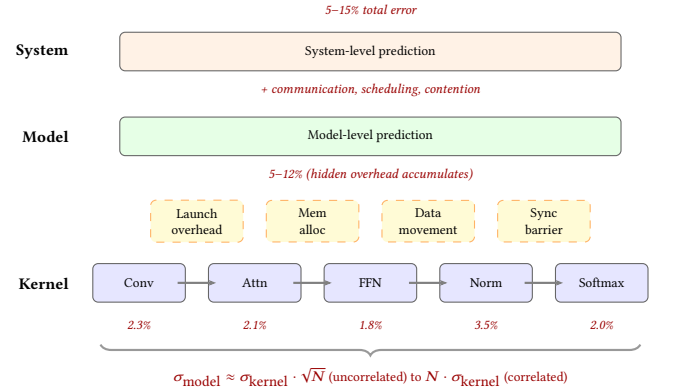
## 7.8 Threats to Validity

**External validity.** Our venue-focused search (ACM DL, IEEE Xplore, arXiv) may under-represent industry publications, workshop papers, and tools distributed only as code repositories without accompanying papers. We exclude proprietary tools (Nsight Compute [56], internal TPU models) from evaluation, though these are arguably the most widely used in practice. The Apple M2 Ultra evaluation platform lacks discrete GPUs, preventing independent D1 verification; all D1 scores are therefore capped at Medium, which may underrate tools whose accuracy claims would survive hardware validation.

**Internal validity.** Our evaluation covers 5 of 22 surveyed tools, selected for methodology diversity (one per methodology type). While this ensures breadth, it means that findings about specific methodology types rest on single tool instances—e.g., our assessment of ML-augmented approaches relies entirely on nn-Meter, which may be unrepresentative due to its unusually poor deployment quality. A complete study would add SimAI (trace-driven, NCCL-level), AMALI (analytical, GPU), and Habitat (hybrid, cross-GPU transfer) to strengthen within-category conclusions.

**MTAP-specific concerns.** The MTAP framework introduces three potential biases. *First*, dimension weights ( $w = 0.4, 0.2, 0.2, 0.1, 0.1$ ) reflect our assessment of practitioner priorities; alternative weightings would shift relative rankings, though our sensitivity analysis shows ordinal stability across three weight schemes. *Second*, the D2 (Compositional Fidelity) scores are inherently aspirational—since no tool provides validated cross-level composition, this dimension distinguishes tools primarily by how explicitly they document their scope limitations rather than by measurable composition quality. *Third*, temporal stability assessment (D3 sub-dimension) depends on when the evaluation is conducted: tools that currently succeed may fail under future software stack updates, and our 2024 evaluation captures only a single point in time.

**Construct validity.** MTAP dimensions are designed to be orthogonal, but deployment viability (D4) and temporal stability (a D3 sub-dimension) are mechanistically linked: Docker-based deployment provides temporal stability by freezing dependencies. This correlation means D4 and D3 partially measure the same underlying property (containerization quality), potentially double-counting Docker’s benefits in the composite score.



**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.**

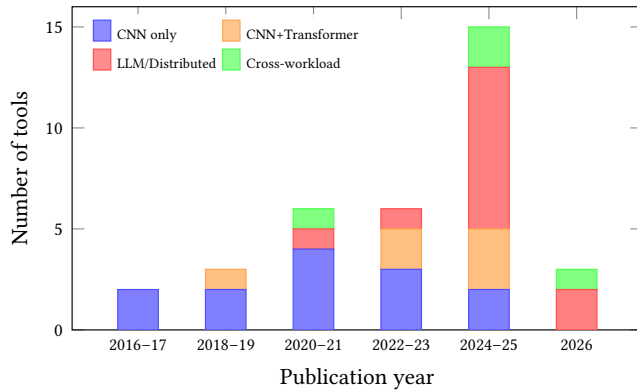
**Measurement validity.** Our evaluation platform (Apple M2 Ultra) lacks discrete GPUs, which restricts D1 assessment to self-reported accuracy analysis. This limitation is partially mitigated by three factors: (1) D2–D5 are fully measurable without target hardware and account for 60% of the composite score; (2) our D1 analysis focuses on structural properties (rank accuracy, error distribution shape, scaling behavior) rather than absolute MAPE, providing insight even without ground-truth measurements; and (3) the M-cap on unverified D1 scores explicitly encodes the epistemic uncertainty, preventing overconfident conclusions. However, a GPU-equipped evaluation would strengthen D1 assessments by enabling independent verification of claimed accuracy figures—potentially changing individual tool scores by up to one grade level (e.g., Medium to High for tools whose claims survive hardware validation, or Medium to Low for tools whose self-reported numbers prove optimistic). We estimate that D1 re-scoring with hardware verification would not change the qualitative finding that deployment methodology dominates accuracy in determining practical utility, since this conclusion rests primarily on D4 and D5 scores, which are hardware-independent.

## 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 ( $\sigma_{\text{model}} \approx \sigma_{\text{kernel}} \cdot \sqrt{N}$  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—analogueous to numerical error analysis—would enable practitioners to reason about end-to-end accuracy from component specifications.





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

**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.

**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 prefill/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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