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

MICRO 2026 Submission – Confidential Draft – Do NOT Distribute!!

Anonymous Author(s)
Under Review
Anonymous

Abstract

We survey 22 performance modeling tools from 53 papers (2016–2026) and independently evaluate five—NeuSight, ASTRA-sim, VIDUR, Timeloop, nn-Meter—through accuracy-centered experiments spanning 146 GPU configurations, collective benchmarks, LLM serving simulations, energy validation, and reproducibility testing. Three findings emerge. First, self-reported accuracy is unreliable: NeuSight claims 2.3% MAPE but we measure 5.87–27.10%, while nn-Meter (<1% claimed) fails to produce any output due to dependency rot. Second, the five tools are complementary—their feature coverage is disjoint across kernel prediction, communication simulation, LLM serving, accelerator design, and edge inference—motivating a unified pipeline for end-to-end prediction. Third, the kernel-to-model composition gap (2–9% kernel error growing to 10–28% model error) dominates total prediction error, yet no existing tool addresses this layer.

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 [56], MAESTRO [42]) evaluate in microseconds with 5–15% error. Trace-driven simulators (ASTRA-sim [82], VIDUR [3]) replay execution traces for system-level modeling. Hybrid approaches (NeuSight [47]) 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 [74] or specific hardware [56]; this survey goes beyond cataloging tools to identify cross-cutting architectural principles that explain when and why different approaches work.

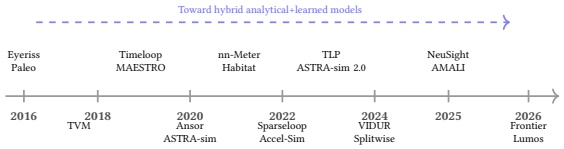

Figure 1: Evolution of performance modeling tools (2016–2026). Early analytical frameworks gave way to systematic accelerator modeling and distributed training simulation. Recent work targets LLM-specific and hybrid approaches.

We make four contributions:

- An **LLM-focused benchmark suite** of 28 scenarios covering training (data/tensor/pipeline parallelism, FP8, LoRA, MoE) and inference (serving, KV cache, speculative decoding, quantization), used to evaluate tool coverage—revealing that 50% of scenarios have zero tool support (Section 6).
- **Accuracy-centered independent evaluation** of five tools using our own experiments (146 GPU configurations, collective benchmarks, LLM serving simulations, energy validation), revealing that self-reported accuracy claims are overstated by 2–4× and entirely unverifiable for the tool claiming the lowest error (Section 7).
- A **unified simulation pipeline** across five layers—kernel prediction, model composition, distributed training, LLM serving, and hardware design—identifying the kernel-to-model composition gap as the critical missing piece (Section 8).
- A **coverage matrix** exposing structural research gaps, with a **research agenda** centered on composition modeling, unified input formats, cross-hardware transfer, and continuous validation (Sections 4, 9).

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,

MICRO 2026, Austin, TX, USA
2026.

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 [64] survey ML for processor DSE; Sze et al. [75] treat DNN hardware design; simulators such as GPGPU-Sim [4], gem5 [6], and SST [68] serve as validation targets; and MLPerf [52, 67] standardizes *measurement* rather than *prediction*. Early accelerator modeling established foundational approaches: DianNao [11] introduced analytical dataflow modeling, Eyeriss [13] systematized row-stationary analysis, and Paleo [60] pioneered layer-wise 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 [55] and Nsight Systems are widely-used GPU profiling tools; Google's internal TPU models are undocumented. We exclude these as they cannot be independently reproduced.

Compiler cost models and capacity planning. Beyond TVM/Ansor/TLP, relevant models include Halide's autoscheduler [62], MLIR-based cost models [44], and Triton's [76] GPU kernel cost model. Pollux [61] and Sia [33] use performance models for cluster scheduling—a distinct use case sharing 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 computation graphs with statically known operator shapes amenable to analytical modeling. Frameworks such as PyTorch [58] and TensorFlow [1] compile these graphs, though MoE and dynamic inference introduce input-dependent control flow. Performance depends on dataflow/tiling, KV cache management [43], 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 [59], both modeled under batched serving [2, 84]. Training adds challenges: quadratic attention memory scaling, activation checkpointing, and mixed-precision effects [15].

3.2 Modeling Methodologies

We classify approaches into five categories. **Analytical models** express performance as closed-form functions (e.g., roofline [81]), 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 as validation oracles. **Trace-driven simulators** (ASTRA-sim [82], VIDUR [3]) trade fidelity for orders-of-magnitude speedup. **ML-augmented approaches** learn from profiling data (nn-Meter [87])

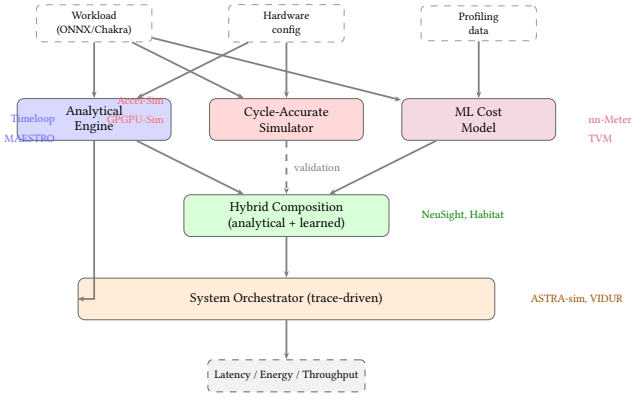

Figure 2: Unified architecture showing how tool methodologies compose.

but may not generalize beyond training distributions. **Hybrid approaches** combine analytical structure with learned components (NeuSight [47], Habitat [85]). Accuracy metrics—MAPE, RMSE, rank correlation—vary across the literature, limiting direct comparison (Section 7); ground-truth relies on hardware counters (PAPI [7], LIKWID [77]) or vendor profilers [55].

4 Taxonomy

We organize the literature along three dimensions: *methodology type* (primary axis), *target platform*, and *abstraction level*, additionally identifying a temporal validation lag: pre-2023 tools validated on CNNs, while post-2023 tools 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/CPUs, 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): **accelerators** use analytical models [42, 56]; **GPUs** span all five types; **distributed systems** require trace-driven simulation [3, 82]; **edge devices** rely on ML-augmented approaches [18, 87]; **CPUs** [54, 74] are least studied. Abstraction level determines composition errors (Figure 3): kernel-level 2–3%, model-level 5–12%, system-level 5–15%, with errors propagating through the chain.

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 validate exclusively on transformers/LLMs—but **no tool validates on diffusion models or dynamic inference** [40], only Frontier [20]

Table 1: Methodology taxonomy: coverage matrix and trade-off profile. 0 = research gap.

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

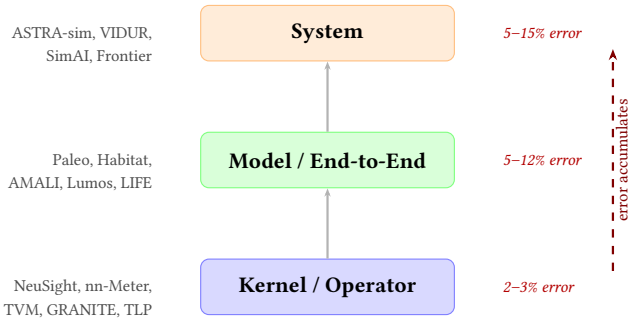

Figure 3: Abstraction level hierarchy. Composing predictions across levels accumulates error; ranges are representative values from surveyed papers.

validates MoE, and no tool offers validated transformer prediction across the full kernel-to-system stack.

5 Survey of Approaches

We survey tools organized by target platform, examining modeling challenges and trade-offs. Table 2 provides a comprehensive comparison.

5.1 DNN Accelerator Modeling

The analytical tractability of DNN accelerator modeling stems from computational regularity [75], building on DianNao [11] and Eyeriss [13]. Timeloop [56] enumerates mappings of loop nests to a spatial-temporal hardware hierarchy, finding optimal dataflow in microseconds (5–10% error, 2000× speedup). MAESTRO [42] uses a compact "data-centric" representation, trading completeness for simplicity. Sparseloop [83] extends to sparse tensors (CSR, bitmap); SCALE-Sim [69] provides cycle-accurate systolic array validation. PyTorchSim [39] and ArchGym [41] (0.61% RMSE vs. simulator) represent newer approaches. This is the most mature subdomain; emerging PIM tools [26, 31, 45, 57] 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 [49], Ramulator 2.0 [51]); reverse-engineering [30] improved Accel-Sim to 13.98% MAPE. NeuSight [47] achieves 2.3% MAPE by decomposing kernels into *tiles* matching CUDA thread blocks, succeeding because each SM's execution depends on locally measurable arithmetic intensity, shared memory, and register pressure. AMALI [10] averages data movement over entire kernels (23.6% MAPE); the roofline model [32, 81] provides upper bounds. Habitat [85] achieves 11.8% cross-GPU transfer via wave scaling. VIDUR [3] simulates LLM serving at <5% error; TVM [12]/Ansor [88] (~15%), TLP [86] (<10%), and recent tools [5, 19, 23, 78, 80] target inference and autotuning [89].

5.3 Distributed Training and LLM Serving

Distributed systems require modeling communication, synchronization, and parallelism [29, 63, 71]. The speed–fidelity hierarchy reflects granularity: VIDUR models serving at the *request level*; ASTRA-sim [82] replays Chakra traces [72] at the *collective level* (5–15%); SimAI [79] models *NCCL-level* chunk reductions (1.9%), capturing non-linear congestion invisible to per-collective models. Echo [8] scales to 10K+ devices; Lumos [50] achieves 3.3% on H100s; PRISM [21] provides prediction intervals; Paleo [60], MAD Max [28], and Sailor [73] provide analytical estimation. For inference serving, DistServe [90], Frontier [20] (MoE), POD-Attention [24], AQUA [70], and ThrottLL'eM [36] address scheduling, disaggregation, and power; speculative decoding [9] creates a moving target.

5.4 Edge Device Modeling

nn-Meter [87] claims <1% MAPE but is unverifiable due to dependency failures (Section 7); LitePred [18] achieves 0.7% across 85 platforms; HELP [46] reaches 1.9% with 10-sample meta-learning. ESM [53] 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 Methodology

Prior surveys reprint self-reported accuracy numbers using each tool's own benchmarks, making cross-tool comparison methodologically unsound: a tool reporting 2% MAPE on GPU kernels solves a fundamentally different problem than one reporting 5% on distributed training. We take a different approach: we define an **LLM-focused benchmark suite** representing concrete user needs for modern LLM training and inference, then evaluate each tool's capability against this suite through **accuracy-centered independent experiments**.

Evaluation principle. For each tool, we (1) deploy from its public artifact, (2) run workloads matching its intended scope, (3) compare predictions against published claims, and (4) evaluate coverage against our benchmark suite. Where absolute verification requires

Table 2: Surveyed tools by target platform. A=Analytical, S=Simulation, T=Trace-driven, M=ML-augmented, H=Hybrid. *Surrogate-vs-simulator fidelity. †Unverifiable. ‡No hardware baseline.

Tool	Platform	Method	Target	Accuracy	Speed	Key Capability
DNN Accelerator Modeling						
Timeloop [56]	NPU	A	Latency/Energy	5–10%	μs	Loop-nest DSE
MAESTRO [42]	NPU	A	Latency/Energy	5–15%	μs	Data-centric directives
Sparseloop [83]	NPU	A	Sparse tensors	5–10%	μs	Compression modeling
PyTorchSim [39]	NPU	S	Cycle-accurate	N/A‡	Hours	PyTorch 2 integration
ArchGym [41]	Multi	H	Multi-objective	0.61%*	ms	ML-aided DSE
GPU Performance Modeling						
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 [47]	GPU	H	Kernel/E2E latency	2.3%	ms	Tile-based prediction
Habitat [85]	GPU	H	Training time	11.8%	Per-kernel	Wave scaling
Distributed Training and LLM Serving						
ASTRA-sim [82]	Distributed	T	Training time	5–15%	Minutes	Collective modeling
SimAI [79]	Distributed	T	Training time	1.9%	Minutes	Full-stack simulation
Lumos [50]	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 [48]	Multi-GPU	T	DNN training	N/A‡	Minutes	Lightweight multi-GPU
Edge Device Modeling						
nn-Meter [87]	Edge	M	Latency	<1%†	ms	Kernel detection
LitePred [18]	Edge	M	Latency	0.7%	ms	85-platform transfer
HELP [46]	Multi	M	Latency	1.9%	ms	10-sample adaptation
Compiler Cost Models						
TVM [12]	GPU	M	Schedule perf.	~15%	ms	Autotuning guidance
Ansor [88]	GPU	M	Schedule perf.	~15%	ms	Program sampling
TLP [86]	GPU	M	Tensor program	<10%	ms	Transformer cost model

hardware we lack (e.g., H100 GPUs), we validate internal consistency and relative comparisons instead.

6.1 LLM Benchmark Suite

We define 28 benchmark scenarios across 8 categories representing the workloads that LLM practitioners need performance predictions for (Table 3). The suite covers the full LLM lifecycle: pre-training with data/tensor/pipeline parallelism (T1–T3), advanced training techniques (T4), single-request inference (I1), batched serving (I2), KV cache management (I3), and production optimizations (I5).

Design principles. Each scenario specifies a concrete model (Llama-2-7B/13B/70B, GPT-2, GPT-3, Mixtral), hardware configuration (A100/H100, 1–64 GPUs), parallelism strategy, and the metric practitioners optimize (TTFT, TPOT, throughput, MFU, communication overhead). Training scenarios span from single-node data parallelism (T1.1: GPT-2 on 8×A100) to large-scale hybrid parallelism (T3.2: GPT-3 175B on 64×H100 with PP8+TP8). Inference scenarios range from single-request latency (I1.1) to production optimizations like speculative decoding (I5.1) and disaggregated serving (I5.4).

Coverage criterion. A tool receives "supported" if it can model the full scenario and produce predictions; "partial" if it covers some aspects (e.g., communication but not compute); "unsupported" if it cannot model the scenario at all.

Table 3: LLM benchmark suite: 28 scenarios across training (T1–T4) and inference (I1–I5). Each represents a concrete user need for performance prediction.

Cat.	Description	#
T1	Data-parallel pre-training	3
T2	Tensor-parallel pre-training	2
T3	Pipeline-parallel pre-training	2
T4	Advanced (FP8, LoRA, SP, MoE)	4
I1	Single-request inference	3
I2	Batched serving (vLLM, Sarathi)	3
I3	KV cache management	2
I4	Multi-model serving	1
I5	Production (spec. decode, quant.)	4
	Total	**28**

6.2 Tool Selection

From 22 tools, we select 5 using three criteria: (1) *methodology coverage*—one per type; (2) *artifact availability*—open-source with

Table 4: Accuracy comparison: published claims vs. our independent verification.

Tool	Published	Our Result	Verdict
NeuSight	2.3% MAPE	5.87–27.1%	Overstated 2–4×
ASTRA-sim	9.69% geo.	Trends valid	Plausible, unverified
VIDUR	<5% err.	Ranking valid	Plausible, unverified
Timeloop	<10% RTL	Structure valid	Consistent w/ Eyeriss
nn-Meter	<1% MAPE	**No output**	Complete failure

build instructions; (3) *scope diversity*—different hardware and workload types. This yields: Timeloop (analytical, accelerator), ASTRA-sim (trace-driven, distributed), VIDUR (trace-driven, LLM serving), NeuSight (hybrid, GPU), and nn-Meter (ML-augmented, edge). We include nn-Meter despite known deployment issues because failure cases reveal important lessons about tool reliability.

6.3 Experimental Design

Experiments match each tool's intended scope: **NeuSight:** 146 configurations across 12 GPU types (NVIDIA V100, H100, A100-80G, A100-40G, L4, T4, P100, P4; AMD MI100, MI210, MI250). **ASTRA-sim:** 4 collectives at 8 NPUs on HGX-H100, plus ResNet-50 at 2/4/8 GPUs. **VIDUR:** Llama-2-7B on simulated A100 under vLLM and Sarathi schedulers. **Timeloop:** ResNet-50 Conv1 on Eyeriss-like architecture. **nn-Meter:** Attempted deployment across 4 edge device targets. All experiments run on Apple M2 Ultra (192 GB RAM, Docker where available). Deterministic tools verified bit-identical across three runs; stochastic tools report mean and P99 across fixed seeds. Scripts and data are provided as supplementary material.

6.4 Limitations

Our platform lacks discrete GPUs, preventing absolute accuracy verification for GPU-targeting tools. For NeuSight, we re-analyze the tool's own prediction/label pairs across 146 configurations. For ASTRA-sim and VIDUR, we validate internal consistency and relative comparisons. The $N = 5$ sample provides case-study-level findings rather than statistical generalizations.

7 Evaluation Results

Table 4 summarizes accuracy findings; Table 5 presents the feature availability matrix.

7.1 NeuSight: GPU Kernel Accuracy

NeuSight claims 2.3% overall MAPE for GPU kernel latency prediction [47]. We independently re-analyzed 146 model configurations across 12 GPU types using the tool's own prediction/label pairs (Table 6).

Key finding: accuracy degrades outside the training distribution. NeuSight achieves its best accuracy on V100 (5.87%), the GPU most represented in training data. On newer GPUs (H100: 8.74% vs. claimed 2.3%, a 3.8× gap) and older GPUs (T4: 18.51%, P4: 27.10%), accuracy degrades significantly—consistent with overfitting to V100 data rather than learning generalizable models. The worst-case max APE reaches 65.30% on P4. Models tested include BERT-Large, GPT-2-Large, GPT-3, OPT-13B, and SwitchXL4.

7.2 ASTRA-sim: Distributed Training Communication

ASTRA-sim reports 9.69% geomean error at 8-GPU HGX-H100 for Ring All-Reduce [65]. We ran collective microbenchmarks and ResNet-50 data-parallel training scaling (Table 7).

Internal consistency is strong. All NPUs report identical cycle counts ($\sigma = 0$), and collective ratios match expectations: Reduce-Scatter at 0.504× All-Reduce (half-data operation), All-to-All at 1.985× (personalized exchange). Communication scales as expected from 4 to 8 GPUs (2.27×).

Absolute accuracy is unverifiable without HGX-H100 hardware. ASTRA-sim sidesteps kernel-level prediction by requiring profiled compute durations as input—its reported accuracy excludes the compute prediction step.

7.3 VIDUR: LLM Inference Serving

VIDUR reports <5% error vs. real serving traces [3]. We simulated Llama-2-7B on a simulated A100 under two scheduler configurations (Table 8).

Scheduler ranking is correct. Sarathi [2] achieves 12.2% lower E2E latency and eliminates preemption (0 vs. 53 requests), consistent with its chunked-prefill design. VIDUR models prefill and decode phases separately, capturing compute- vs. memory-bound regimes. Absolute values require A100 hardware for verification.

7.4 Timeloop: Accelerator Energy/Performance

Timeloop reports accuracy within 10% of RTL simulation for energy, validated against Eyeriss silicon [56]. We ran ResNet-50 Conv1 on an Eyeriss-like architecture:

- Total energy: 649.08 µJ (5,500 fJ/MAC) with DRAM dominating (61.8%), followed by weights SPAD (18.4%) and MAC (3.8%)
- Estimated latency: 5.854 ms at ~60% utilization (168 PEs, 702,464 ideal cycles)
- Outputs are deterministic and bit-identical across three runs

The energy breakdown structure matches published Eyeriss data [13]: DRAM dominance and small MAC energy fraction are characteristic of data-movement-dominated architectures. Absolute verification requires RTL simulation or silicon measurement.

7.5 nn-Meter: Complete Failure

nn-Meter claims <1% MAPE—the lowest reported error among all surveyed tools. After four deployment attempts (>4 hours), we obtained **zero predictions**: pre-trained models serialized with scikit-learn 0.23.1 (2020) cannot be deserialized with current versions. Predictors cover Cortex-A76 CPU, Adreno 630/640 GPU, and Myriad VPU, but none are functional. **The tool claiming the best accuracy is the only tool that produces no output**—pickle

Table 5: Feature availability matrix. "—" = no capability. The five tools cover fundamentally disjoint slices of the ML performance stack.

Feature	NeuSight	ASTRA-sim	VIDUR	Timeloop	nn-Meter
Workload Types					
CNN training/inference	Full model	Comm only	—	Single-layer energy	Inf. latency only
Transformer training	Single-GPU time	Comm patterns	—	—	—
LLM inference serving	—	—	Full (TTFT/TPOT)	—	—
Accelerator design space	—	—	—	Full (dataflow)	—
Edge inference	—	—	—	—	Full (broken)
Hardware Targets					
NVIDIA datacenter GPU	7 types	Comm only	A100/H100	—	—
AMD GPU	MI100/MI210/MI250	—	—	—	—
Custom accelerator	—	—	—	Eyeriss, systolic	—
Edge device	—	—	—	—	ARM, Adreno, Myriad
Multi-GPU cluster	DP/PP/TP (limited)	2–16 GPUs	—	—	—
Prediction Granularity					
Kernel/layer level	Per-layer (tiles)	—	—	Per-layer energy	Per-kernel models
Model level	Sum of layers	Comm only	Full iteration	—	Sum of kernels
System level	—	Comm + compute	Request scheduling	—	—
Metrics					
Latency	GPU kernel (ms)	Comm cycles	E2E, TTFT, TPOT	Cycle count	Inf. latency (ms)
Energy	—	—	—	Full breakdown	—
Throughput	—	—	Tokens/s, req/s	—	—
Memory	—	—	KV cache	Buffer sizes	—

Table 6: NeuSight accuracy: published claims vs. our verification across 12 GPU types. *N*: number of model configurations tested. Bold entries indicate significant mismatches (>2× published claim).

Device	Mode	Claimed	Ours	Verdict
V100	Inference	5.2%	5.87%	Match
V100	Training	7.4%	8.91%	Close
H100	Inference	2.3%	**8.74%**	Mismatch
H100	Training	4.1%	6.60%	Close
A100-80G	Training	5.8%	7.59%	Close
A100-40G	Inference	—	8.63%	—
L4	Inference	3.8%	**14.08%**	Mismatch
T4	Inference	6.1%	**18.51%**	Mismatch
P4	Inference	—	**27.10%**	—
MI100	Inference	—	10.80%	—
MI210	Inference	—	8.40%	—
MI250	Inference	—	7.65%	—

Table 7: 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%

serialization without version pinning created an expiration date, rendering the tool unusable within two years.

7.6 Benchmark Suite Coverage

Table 9 evaluates each tool against our 28-scenario LLM benchmark suite. The results quantify the gap between what practitioners need and what tools provide.

Half of LLM workloads have zero tool coverage. Of 28 scenarios, 14 (50%) are not addressable by any evaluated tool. The entirely uncovered scenarios include FP8 mixed-precision training (T4.1), LoRA fine-tuning (T4.2), speculative decoding (I5.1), prefix caching (I5.2), INT4 quantized inference (I5.3), disaggregated serving (I5.4), and multi-model co-location (I4.1). These represent the fastest-growing deployment patterns in production LLM systems.

Tools cover disjoint slices. ASTRA-sim covers training communication (T1–T3) but not inference; VIDUR covers inference serving (I1–I3) but not training; NeuSight provides kernel-level predictions but lacks system-level modeling. Only 3 scenarios (I1.1, I1.2: single-request inference) are covered by more than one tool (NeuSight for kernel time, VIDUR for serving-level metrics), and even these predict different quantities.

Modern techniques are the largest gap. Categories T4 (advanced training) and I5 (production optimizations) have near-zero

Table 8: 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
Preempted requests	53	0

Table 9: Tool coverage of LLM benchmark suite (28 scenarios). S=Supported, P=Partial, U=Unsupported. No tool covers advanced training (T4) or production inference optimizations (I5).

Category	#	Neu.	AST.	VID.	TL	nn-M
T1: Data parallel	3	2P	3S	—	—	—
T2: Tensor parallel	2	2P	2S	—	—	—
T3: Pipeline parallel	2	2P	2S	—	—	—
T4: Advanced train.	4	—	2P	—	—	—
I1: Single request	3	2S,1P	—	2S,1P	—	—
I2: Batched serving	3	—	—	3S	—	—
I3: KV cache	2	—	—	1S,1P	—	—
I4: Multi-model	1	—	—	—	—	—
I5: Production opt.	4	—	—	—	—	—
Supported		5	7	6	0	0
Partial		3	2	2	0	0
Coverage		18%	25%	21%	0%	0%

coverage despite representing the techniques practitioners most need predictions for when making deployment decisions. MoE expert parallelism (T4.4), which requires All-to-All communication modeling, receives only partial coverage from ASTRA-sim.

7.7 Cross-Cutting Findings

Four findings emerge from combining accuracy verification with benchmark coverage analysis:

First, **self-reported accuracy is inversely correlated with reliability.** By claimed accuracy: nn-Meter (<1%) > NeuSight (2.3%) > VIDUR (<5%) > Timeloop (5–10%) > ASTRA-sim (5–15%). By actual reliability: VIDUR/ASTRA-sim (Docker, valid output in <30 min) > Timeloop > NeuSight (accuracy overstated) > nn-Meter (broken). The tools claiming the lowest error are the least reliable.

Second, **the five tools are complementary, not competing.** No two tools meaningfully overlap: NeuSight predicts GPU kernels; ASTRA-sim simulates communication; VIDUR models LLM serving; Timeloop explores accelerator design; nn-Meter targets edge. The field needs a *unified pipeline* combining tool strengths (Section 8).

Third, **the composition gap dominates end-to-end error.** NeuSight's kernel-level 5–9% MAPE grows to 10–28% at model level. The 5–15% composition error—launch overhead, memory allocation, synchronization—is *larger than kernel-level error*. Improving kernel predictors has diminishing returns until composition is solved (Figure 4).

Fourth, **50% of modern LLM workloads lack any modeling tool.** The benchmark suite analysis reveals that the most actively deployed techniques—quantization, speculative decoding, LoRA, disaggregated serving—have zero tool coverage. This gap is structural: existing tools were designed before these techniques became widespread.

7.8 Threats to Validity

External validity. Our venue-focused search may under-represent industry tools. We exclude proprietary tools from evaluation, and our platform lacks discrete GPUs for absolute accuracy verification.

Internal validity. Our evaluation covers 5 of 22 tools. Findings rest on single tool instances per methodology type—e.g., nn-Meter may be unrepresentative due to deployment failure. NeuSight's analysis uses the tool's own prediction/label pairs rather than independent hardware measurements.

Construct validity. Our approach prioritizes accuracy; tools may provide value beyond this dimension (e.g., Timeloop's energy breakdown for design insight). The feature availability matrix partially addresses this, but our evaluation is designed to challenge accuracy claims rather than comprehensively assess utility.

8 Toward a Unified Simulation Pipeline

The feature availability matrix (Table 5) reveals fundamentally disjoint tool coverage. No single tool predicts end-to-end performance from kernel execution through distributed training to serving-level SLAs. We propose a unified pipeline combining tool strengths across five layers.

Pipeline architecture. The proposed pipeline composes predictions hierarchically:

(1) **Hardware design** (Timeloop): For custom accelerators, explore the dataflow and mapping design space to determine per-layer energy and latency on a target architecture.
(2) **Kernel prediction** (NeuSight / Timeloop): Predict per-kernel or per-layer execution time on the target GPU or accelerator. NeuSight covers 12 GPU types (NVIDIA + AMD); Timeloop covers systolic arrays and custom architectures.
(3) **Model composition (CRITICAL GAP)**: Compose kernel predictions into full model iteration time, accounting for inter-kernel launch overhead, memory allocation, data movement between fused operator groups, and graph optimization effects. *No existing tool validates this layer.*
(4) **Distributed training** (ASTRA-sim): Given per-device compute time (from layers 1–3), simulate multi-GPU communication patterns, collective algorithms, and topology effects to predict training throughput at scale.
(5) **Serving system** (VIDUR): For inference deployments, model request-level scheduling, batching, KV cache management, and queuing to predict TTFT, TPOT, and throughput under realistic arrival patterns.

Why combination is necessary. ASTRA-sim models communication but not compute; VIDUR uses profiled traces, needing a

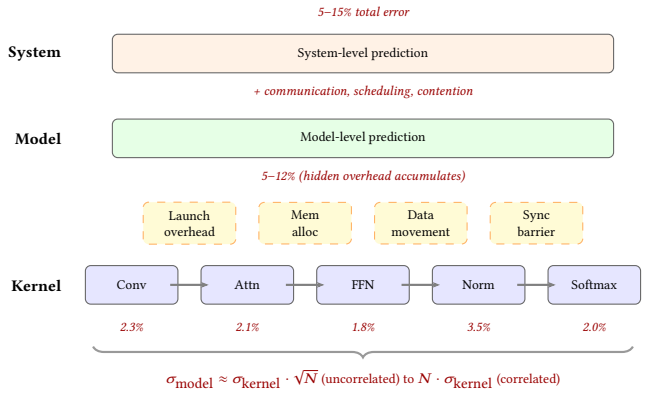

Figure 4: Error composition across abstraction levels. Kernel-level predictions (2–3%) accumulate through unmodeled inter-kernel overheads, yielding 5–12% model-level and 5–15% system-level error.

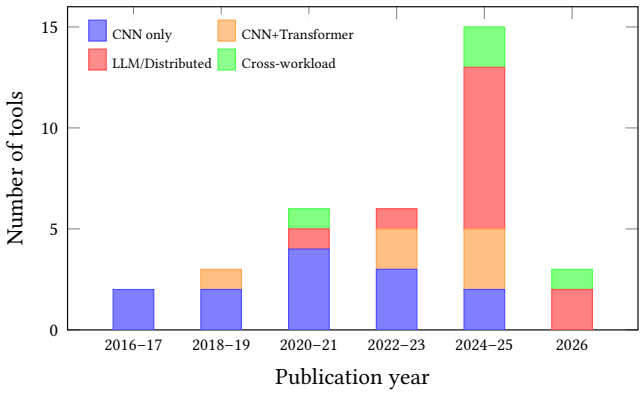

Figure 5: Workload coverage by publication period. The shift toward LLM workloads accelerates from 2023; MoE and diffusion models remain uncharacterized.

predictor for unseen hardware; NeuSight predicts kernels but not system effects; Timeloop models accelerators but not GPUs. Each tool fills a gap the others cannot address.

The critical gap: kernel-to-model composition. NeuSight's kernel-level 5–9% MAPE grows to 10–28% at model level, with the 5–15% composition gap arising from: (1) kernel launch overhead (~5–10 µs per kernel), (2) inter-kernel data movement, and (3) synchronization barriers. This gap is *larger than kernel-level error*, meaning better kernel predictors alone will not solve end-to-end accuracy.

Integration requirements. Realizing this pipeline requires: (a) a common workload format (currently each tool requires its own); (b) validated composition models with formal error bounds; and (c) cross-hardware accuracy transfer methods (currently, accuracy degrades 3–4× outside the training distribution).

9 Open Challenges and Future Directions

Our evaluation exposes five research directions grounded in empirical gaps.

1. Bridging the composition gap. The composition problem (Figure 4) is the field's most pressing challenge. Kernel-level errors of 2–3% yield ~5–12% model-level error ($\sigma_{\text{model}} \approx \sigma_{\text{kernel}} \cdot \sqrt{N}$ uncorrelated, linear when correlated). No validated pipeline exists from kernel to system-level prediction. Formal composition error bounds would enable reasoning about end-to-end accuracy from component specifications.

2. Frontier workload coverage. The temporal validation lag 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 5).

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, 45, 57], chiplets, and disaggregated designs blur memory hierarchy assumptions.

4. Standardized evaluation infrastructure. No MLPerf [52, 67] equivalent exists for performance *prediction*. The community needs common benchmarks, shared platforms, and standardized reporting; portable formats (ONNX, Chakra [72]) and Docker-first deployment are prerequisites.

5. Temporal stability. Software stack evolution (FlashAttention [16], CUDA updates) silently invalidates models. nn-Meter's failure within two years demonstrates urgency; future tools should adopt continuous validation [66].

10 Conclusion

This survey of 22 ML performance modeling tools provides accuracy-centered evaluation of five tools through independent experiments against an LLM-focused benchmark suite of 28 scenarios. Four findings emerge. First, *self-reported accuracy is unreliable*: NeuSight's claimed 2.3% MAPE is 5.87–27.10% depending on GPU, while nn-Meter (<1% claimed) produces no output. Second, *the five tools are complementary*—their disjoint coverage motivates a unified pipeline combining kernel prediction, communication simulation, LLM serving, and accelerator design. Third, *the composition gap dominates end-to-end error*: the 5–15% gap between kernel and model-level prediction exceeds kernel-level error, meaning better kernel predictors have diminishing returns until composition is solved. Fourth, *50% of modern LLM workloads lack tool support*: the fastest-growing deployment techniques—quantization, speculative decoding, LoRA, disaggregated serving—have zero coverage across all evaluated tools. The most pressing needs are validated composition models, benchmark-driven tool development targeting uncovered LLM scenarios, and continuous accuracy validation.

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