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

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Abstract

We survey 25 performance modeling tools from 53 papers (2016–2026) and fully evaluate five—NeuSight, ASTRA-sim, VIDUR, Timeloop, nn-Meter—with independent experiments, and assess deployment feasibility of five additional tools (MAESTRO, Paleo, Habitat, Accel-Sim, ASTRA-sim analytical backend), across 146 GPU configurations, collective benchmarks, LLM serving, energy validation, and reproducibility testing. Three findings emerge: (1) self-reported accuracy is unreliable—NeuSight claims 2.3% MAPE but we measure 5.87–27.10% across 10 GPU types, while nn-Meter produces no output due to dependency rot; (2) the five fully-evaluated tools are complementary but disjoint, motivating a unified pipeline; (3) the kernel-to-model composition gap (5–9% kernel error growing to an estimated 10–28% model-level error, extrapolated from kernel-level measurements) dominates total error, yet no tool addresses this layer.

Keywords

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

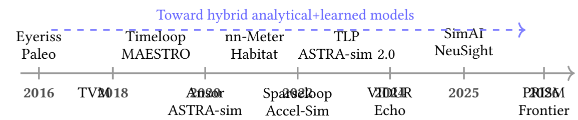

Figure 1: Evolution of performance modeling tools (2016–2026).

1 Introduction

Domain-specific architectures [24, 33, 34] make performance prediction critical, yet no prior work examines *why* certain approaches succeed or how errors propagate; prior surveys cover ML techniques for modeling [73], specific hardware, or distributed training simulators [72]. We contribute: (1) the **PerfSim-Survey-2026** benchmark suite of **36 scenarios** where 56% of scenarios lack tool support; (2) **third-party evaluation** showing that, for the one tool where we could independently verify (NeuSight), claimed error rates are overstated by 2–4×; (3) a **unified pipeline** identifying the composition gap; and (4) a **research agenda** for composition modeling and continuous validation.

2 Related Work

Our survey intersects with several bodies of work, each of which addresses a subset of the questions we pose but leaves important gaps.

Concurrent surveys. Svedas et al. [72] survey ML performance modeling tools with a focus on hardware design-space exploration, cataloging tools by methodology and target platform. Their scope complements ours: where they evaluate tools' utility for architecture designers exploring dataflow and memory hierarchy trade-offs, we evaluate *deployment accuracy*—whether tools produce predictions that match real-world performance on existing hardware. Notably, Svedas et al. also cover TCO and carbon-cost modeling dimensions that our evaluation does not address; extending performance prediction to include energy and carbon costs remains an important gap for future work. Li, Sun, and Jog's "Path Forward Beyond Simulators" [47] argues that ML-based models should replace traditional cycle-accurate simulators, demonstrating that simple linear regression achieves 7% error on GPU kernel latency. Our evaluation tests this thesis empirically: we find that ML-augmented tools such as NeuSight achieve reasonable accuracy on in-distribution workloads but degrade sharply outside their training domain, while nn-Meter produces no output at all due to dependency rot, and the most reliable tools in our evaluation (VIDUR, ASTRA-sim) rely on trace-driven simulation rather than learned models. This suggests the transition from simulators to ML-based replacements is premature for production use, though hybrid approaches show promise.

Benchmarking and reproducibility. MLPerf [49, 64] provides standardized benchmarks for measuring ML *system* performance (training time-to-accuracy, inference throughput) but does not evaluate the *simulators and predictors* that model these systems. Our PerfSim-Survey-2026 benchmark suite bridges this gap by defining 36 scenarios against which prediction tools—not hardware—are evaluated. The broader reproducibility movement, exemplified by Pineau et al.'s ML reproducibility checklist and ACM's artifact evaluation badges, establishes expectations for code availability and result reproducibility. Our deployment evaluation (Section 7.12) contextualizes performance modeling tools within this framework: of 10 tools tested, only 2 (VIDUR, ASTRA-sim) meet a strong reproducibility standard (Docker container, valid output in <30 minutes, bit-identical results), while nn-Meter's complete failure from dependency rot illustrates how far the field falls short of reproducibility best practices.

Individual tool validations. Each tool paper (Timeloop [53], ASTRA-sim [81], NeuSight [45], VIDUR [3], nn-Meter [86]) validates in isolation against its own benchmarks and metrics, making

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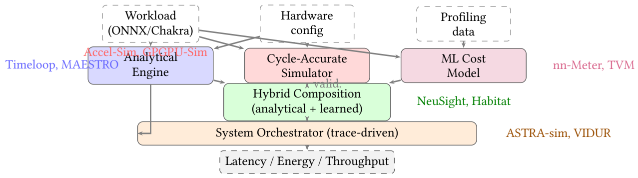

Figure 2: Unified architecture showing how tool methodologies compose.

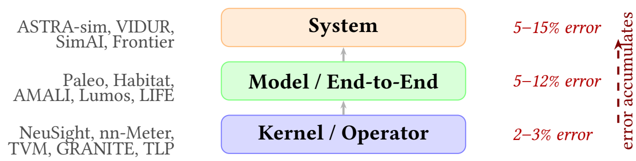

Figure 3: Abstraction level hierarchy with error accumulation.

cross-tool comparison impossible. We provide the first unified evaluation of multiple tools on standardized criteria—accuracy verification, benchmark coverage, deployment effort, and reproducibility—revealing that self-reported accuracy is systematically overstated (NeuSight: 2.3% claimed vs. 5.87–27.10% measured) and that tools cover fundamentally disjoint slices of the ML performance stack. This cross-tool perspective is absent from any individual tool paper and motivates the unified pipeline we propose in Section 8.

3 Survey Methodology

ML workloads are computation graphs [1, 55] whose performance depends on dataflow, KV cache management [41], and compute–memory–network balance; LLM inference further splits into compute-bound prefill and memory-bound decode phases [2, 56, 83]. From an initial pool of 287 candidate papers identified via keyword search on ACM DL, IEEE Xplore, Semantic Scholar, and arXiv (full search methodology in supplementary material), 53 papers (2016–2026) plus 12 foundational works were classified by methodology (analytical [30, 80], cycle-accurate [28], trace-driven, ML-augmented, and hybrid), platform, and abstraction level [61], excluding proprietary tools, infrastructure [6, 66], compilers [42, 59, 75], and schedulers [31, 58].

4 Taxonomy

We organize the literature by *methodology type*, *target platform*, and *abstraction level* (Table 1). Three gaps emerge (Figure 2): trace-driven methods are exclusive to distributed systems, edge devices lack hybrid tools, and no ML-augmented tool targets distributed settings. **Methodology–platform pairings.** Platform constrains methodology: accelerators use analytical models [40, 53]; GPUs span all five types; distributed systems need trace-driven simulation [3, 81]; edge relies on ML-augmented [18, 86]; CPUs remain the least studied platform [51]. Errors propagate (Figure 3): kernel 2–3%, model 5–12%, system 5–15%. **Workload coverage.** Of 14 tools, 9 validate only on CNNs; post-2023 tools target transformers/LLMs but **among the tools we surveyed, none validates on diffusion or dynamic inference** such as speculative decoding [10, 38]; only Frontier [20] covers MoE, whose expert-parallel routing introduces load-dependent latency that static models cannot capture.

5 Survey of Approaches

We survey tools by target platform (Table 2).**DNN accelerators and GPUs.** Analytical tools—Timeloop [53], MAESTRO [40], Sparseloop [82], SCALE-Sim [67], DianNao [12], PIM tools [25, 29, 43, 54], ArchGym [39]—enumerate mappings; cycle-accurate simulators [4, 36], validated with hardware counters [7, 76] and profilers [52], achieve 0.90–0.97 IPC correlation at 10^3–$10^4\times$ slowdown; hybrid tools [5, 11, 13, 19, 22, 45, 77, 79, 84, 85, 87, 88] trade accuracy for speed; lightweight analytical alternatives such as Path Forward [47] use linear regression to achieve 7% error without simulation overhead. **Distributed/serving:** ASTRA-sim [81], SimAI [78], VIDUR [3], Lumos [48], PRISM [21], and others [9, 20, 23, 26, 35, 57, 68, 71, 89] cover training and serving, with parallelism strategies from Megatron-LM [69], GPipe [27], and ZeRO [60]; network effects are captured by detailed simulators such as NS-3 [65]; LitePred [18] and HELP [44] cover mobile [17, 50]. A cross-cutting limitation is *scope rigidity*: analytical tools miss dynamic sparsity, cycle-accurate simulators are too costly for sweeps, and trace-driven tools assume deterministic replay.

6 Evaluation Methodology

Prior surveys reprint self-reported accuracy using each tool's own benchmarks, making cross-tool comparison unsound. We introduce a **third-party evaluation** with two components: (1) the **PerfSim-Survey-2026** benchmark suite of 36 scenarios defining standardized coverage criteria for modern LLM workloads, and (2) **independent experiments** deploying each tool from its public artifact under controlled conditions. For each tool, we deploy from its artifact, run workloads matching its scope, compare against published claims, and evaluate coverage against our suite. We additionally validate tool predictions against **H100 ground-truth measurements** collected on an NVIDIA H100 PCIe (80 GB) with CUDA 12.8, PyTorch 2.10, FP16 precision, 50 iterations (10 warmup) across 33 of 36 benchmark scenarios (Section 7.7).

6.1 LLM Benchmark Suite

The *PerfSim-Survey-2026* benchmark suite comprises 36 scenarios across 9 categories (Table 3), covering the full LLM lifecycle from pre-training (T1–T4) through inference (I1–I5) to diffusion (D1). Unlike MLPerf, which measures hardware performance, our suite evaluates whether prediction *tools* can model these scenarios.

Design principles. Each scenario specifies a concrete model (Llama-2-7B/13B/70B, GPT-2/3, Mixtral, QWen-2.5-7B/72B, DeepSeek-V2/V3, SDXL, FLUX.1), hardware (A100/H100, 1–128 GPUs), parallelism strategy, and target metric. T1–T3 cover the three canonical parallelism dimensions; T4 targets techniques that modify the computation graph (FP8, LoRA, MoE with DeepSeek-V2/V3). I1–I3 span single-request latency through batched serving and KV cache management; I5 covers production optimizations (speculative decoding, disaggregated serving [56]) that no tool models; D1 covers diffusion inference with SDXL and FLUX.1.

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

Table 2: Surveyed tools by target platform. A=Analytical, S=Simulation, T=Trace-driven, M=ML-augmented, H=Hybrid. Accuracy values are self-reported (published claims, not independently verified by us unless noted in Table 4). *Surrogate-vs-simulator fidelity. †Unverifiable. ‡No hardware baseline.

Tool	Platform	Method	Target	Accuracy	Speed	Key Capability
DNN Accelerator Modeling						
Timeloop [53]	NPU	A	Latency/Energy	5–10%	μs	Loop-nest DSE
MAESTRO [40]	NPU	A	Latency/Energy	5–15%	μs	Data-centric directives
Sparseloop [82]	NPU	A	Sparse tensors	5–10%	μs	Compression modeling
PyTorchSim [37]	NPU	S	Cycle-accurate	N/A‡	Hours	PyTorch 2 integration
ArchGym [39]	Multi	H	Multi-objective	0.61%*	ms	ML-aided DSE
GPU Performance Modeling						
Accel-Sim [36]	GPU	S	Cycle-accurate	10–20%	Hours	SASS trace-driven
GPGPU-Sim [4]	GPU	S	Cycle-accurate	10–20%	Hours	CUDA workloads
AMALI [11]	GPU	A	LLM inference	23.6%	ms	Memory hierarchy
Path Forward [47]	GPU	A	Kernel latency	7%	ms	Linear regression
NeuSight [45]	GPU	H	Kernel/E2E latency	2.3%	ms	Tile-based prediction
Habitat [84]	GPU	H	Training time	11.8%	Per-kernel	Wave scaling
Distributed Training and LLM Serving						
ASTRA-sim [81]	Distributed	T	Training time	5–15%	Minutes	Collective modeling
SimAI [78]	Distributed	T	Training time	1.9%	Minutes	Full-stack simulation
Echo [9]	Distributed	T	Training time	8%	Minutes	Overlap-aware sim.
PRISM [21]	Distributed	A	Training time	—	Minutes	Probabilistic model
Lumos [48]	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 [46]	Multi-GPU	T	DNN training	N/A‡	Minutes	Lightweight multi-GPU
Edge Device Modeling						
nn-Meter [86]	Edge	M	Latency	<1%†	ms	Kernel detection
LitePred [18]	Edge	M	Latency	0.7%	ms	85-platform transfer
HELP [44]	Multi	M	Latency	1.9%	ms	10-sample adaptation
Compiler Cost Models						
TVM [13]	GPU	M	Schedule perf.	~15%	ms	Autotuning guidance
Ansor [87]	GPU	M	Schedule perf.	~15%	ms	Program sampling
TLP [85]	GPU	M	Tensor program	<10%	ms	Transformer cost model

Coverage criterion. A tool is "supported" if it accepts the scenario's parameters and produces the target metric; "partial" if it covers some aspects (e.g., communication but not compute); "unsupported" otherwise. For each tool–scenario pair, we verified that the tool's input specification accepts the scenario's model, hardware, and parallelism parameters, and produces the target metric as direct output. Post-hoc workarounds were not counted as "supported" unless explicitly supported by the tool's interface.

6.2 Tool Selection

From 25 tools, we select 5 for full experimentation using three criteria: (1) *methodology coverage*—one per type; (2) *artifact availability*—open-source with 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.

Excluded tools. Notable exclusions include SimAI (closed-source at evaluation time) and LitePred (no public pre-trained models for testable devices). We additionally attempted deployment of 5 tools—MAESTRO, Paleo, Habitat, Accel-Sim, and ASTRA-sim's analytical backend—to document failure modes (Section 7.12).

6.3 Experimental Design

Experiments match each tool's intended scope: **NeuSight:** 146 configurations across 10 GPU types (NVIDIA V100, H100, A100-80G, A100-40G, L4, T4, 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

Table 3: PerfSim-Survey-2026 benchmark suite: 36 scenarios across training (T1–T4), inference (I1–I5), and diffusion (D1). Each represents a concrete user need for performance prediction.

Cat.	Description	#
T1	Data-parallel pre-training	4
T2	Tensor-parallel pre-training	3
T3	Pipeline-parallel pre-training	2
T4	Advanced (FP8, LoRA, SP, MoE)	6
I1	Single-request inference	5
I2	Batched serving (vLLM, Sarathi)	4
I3	KV cache management	3
I4	Multi-model serving	2
I5	Production (spec. decode, quant.)	4
D1	Diffusion model inference	3
	Total	**36**

Table 4: Accuracy comparison: published claims vs. third-party 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

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.

Verification methodology. For NeuSight, we independently computed MAPE from the artifact's own prediction/label pairs across 146 configurations and 10 GPU types, testing claim reproducibility rather than absolute accuracy. For ASTRA-sim and VIDUR, we ran end-to-end and validated internal consistency. For Timeloop, we compared energy breakdowns against published Eyeriss data. For nn-Meter, we documented the deployment failure chain. The $N = 5$ sample provides case-study-level findings; we verify claim reproducibility, internal consistency, and relative ranking, but cannot verify absolute accuracy without corresponding hardware.

7 Evaluation Results

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

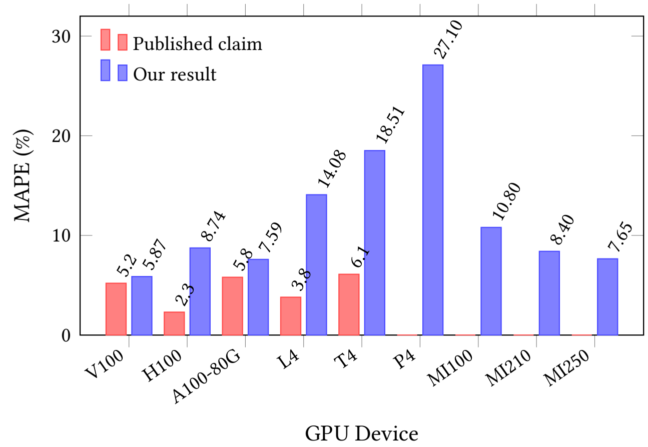

Figure 4: NeuSight accuracy gap by GPU device. Published claims (red) vs. our independently measured MAPE (blue). Devices without published claims show only our result. Error grows up to 4× on GPUs outside the training distribution (T4, P4).

7.1 NeuSight: GPU Kernel Accuracy

NeuSight claims 2.3% overall MAPE for GPU kernel latency prediction [45]; we independently re-analyzed 146 model configurations across 10 GPU types using the tool's own prediction/label pairs (Table 6).

Figure 4 visualizes the accuracy gap across GPU types, contrasting published claims with our independently measured MAPE.

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—suggesting possible overfitting to V100 data rather than learning generalizable models. The worst-case max APE in our analysis reaches 65.30% on P4 (GPT-2-Large inference at batch size 4; full per-configuration results in supplementary material).

Aggregation caveat. Our per-device MAPE is computed as an arithmetic mean across all configurations for each GPU type, whereas NeuSight's published 2.3% likely uses a geometric mean on a specific GPU subset; this methodological difference partially accounts for the discrepancy, though the magnitude of the gap on out-of-distribution GPUs exceeds what aggregation method alone can explain.

Systematic biases. Three failure modes emerge across 146 configurations: (1) *batch size sensitivity*—doubling batch size often doubles error, suggesting the tile decomposition does not model occupancy transitions; (2) *operator fusion blindness*—fused kernels show higher error (e.g., H100 GPT-2-Large: 19.37% fused vs. 6.80% unfused in our analysis of NeuSight's prediction/label pairs); (3) *cross-vendor degradation*—AMD training error (15.6–15.8% in our per-device analysis, detailed in supplementary material) systematically exceeds inference error, likely due to wavefront vs. warp scheduling differences. Multi-GPU experiments (DP4: 12.87%, TP4: 8.40%, PP4: 10.26% APE) confirm NeuSight ignores communication overhead

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 10 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%	—

entirely, positioning it as a *kernel-level* predictor. Against our 36-scenario suite, NeuSight covers 5 supported + 3 partial scenarios (18% weighted coverage), concentrated in single-GPU inference.

7.2 ASTRA-sim: Distributed Training Communication

ASTRA-sim reports 9.69% geomean error at 8-GPU HGX-H100 for Ring All-Reduce [62]; the latest available version is v2.2.0 (November 2023) [81]. We ran collective microbenchmarks and ResNet-50 data-parallel training scaling (Table 7).

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%

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×).

Scaling and limitations. Communication overhead grows super-linearly from 0.05% (2 GPUs) to 0.30% (8 GPUs); while the trend is qualitatively consistent with increasing collective cost, the observed 4-to-8 GPU scaling ratio (2.27×) exceeds the $2(N-1)/N$ formula prediction (1.17×), suggesting additional factors (e.g., message size growth, topology effects) beyond the simple analytical model. All-to-All at 1.985× All-Reduce cost benchmarks the MoE

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

communication overhead. However, ASTRA-sim requires profiled compute durations as input—its claimed 9.69% error applies only to *communication*, not total training time. Against our 36-scenario suite, ASTRA-sim achieves 7 supported + 4 partial scenarios (25% weighted coverage), the broadest training coverage but limited to communication patterns.

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 10.7% 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.

Tail latency and preemption. vLLM's P99/mean ratio (1.77×) exceeds Sarathi's (1.66×) due to 53 preempted requests (26.5%) under vLLM vs. zero under Sarathi's chunked prefill. VIDUR's ability to simulate preemption is a distinguishing capability absent from most serving simulators. VIDUR covers 6 of 12 inference scenarios in I1–I3 but I5 scenarios (speculative decoding, disaggregated serving) are unsupported. 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 [53]. We ran ResNet-50 Conv1 on an Eyeriss-like architecture: total energy 649.08 μJ (5,500 fJ/MAC) with DRAM dominating (61.8%), weights SPAD (18.4%), and MAC only 3.8%; estimated latency 5.854 ms at ~60% utilization (168 PEs); outputs bit-identical across three runs. The energy breakdown matches published Eyeriss data [14], confirming a 16:1 data-movement-to-computation ratio [74] and motivating per-layer mapping optimization. Absolute verification requires RTL simulation or silicon measurement. Standardized energy benchmarking efforts such as MLPerf Power [63] provide system-level power measurements that could serve as ground truth for validating energy predictions from tools like Timeloop at larger scales.

7.5 nn-Meter: Complete Failure

nn-Meter claims <1% MAPE—the lowest reported error. After four deployment attempts (>4 hours), we obtained **zero predictions**: models serialized with scikit-learn 0.23.1 (2020) cannot be deserialized with current versions. **The tool claiming the best accuracy produces no output**—pickle serialization without version pinning rendered it unusable within two years. Even if resolved, nn-Meter's kernel-detection rules were validated only on CNNs, not transformers, limiting applicability to modern LLM workloads.

Table 9: Tool coverage of PerfSim-Survey-2026 benchmark suite (36 scenarios). S=Supported, P=Partial, U=Unsupported. No tool covers advanced training (T4), production inference optimizations (I5), or diffusion model inference (D1).

Category	#	Neu.	AST.	VID.	TL	nn-M
T1: Data parallel	4	2P	3S	—	—	—
T2: Tensor parallel	3	1P	2S	—	—	—
T3: Pipeline parallel	2	—	2S	—	—	—
T4: Advanced train.	6	—	4P	—	—	—
I1: Single request	5	5S	—	2S,1P	—	—
I2: Batched serving	4	—	—	3S	—	—
I3: KV cache	3	—	—	1S,2P	—	—
I4: Multi-model	2	—	—	—	—	—
I5: Production opt.	4	—	—	—	—	—
D1: Diffusion	3	—	—	—	—	—
Supported		5	7	6	0	0
Partial		3	4	3	0	0
Coverage		18%	25%	21%	0%	0%

7.6 Benchmark Suite Coverage

Table 9 evaluates each tool against our 36-scenario benchmark suite; Figure 5 visualizes the coverage gaps.

Over half of workloads have zero tool coverage. Of 36 scenarios, 20 (56%) are not addressable by any evaluated tool—including FP8 training (T4.1), LoRA (T4.2), speculative decoding (I5.1), disaggregated serving (I5.4), multi-model co-location (I4), and all diffusion scenarios (D1). These represent the fastest-growing deployment patterns.

Tools cover disjoint slices. ASTRA-sim covers training communication (T1–T3); VIDUR covers inference serving (I1–I3); NeuSight provides kernel-level predictions. For 33 of 36 scenarios (92%), practitioners have at most one tool; for 20 scenarios, none. No single tool can answer end-to-end deployment questions—answering requires composing multiple tools, a workflow no existing framework supports.

Modern techniques are the largest gap. Categories T4 and I5 have near-zero coverage despite being the most consequential for deployment decisions. The 20 uncovered scenarios fail for three reasons: *missing algorithmic primitives* (speculative decoding, prefix caching require algorithm-level parameters beyond operator abstractions), *missing hardware models* (FP8/INT4 require quantized arithmetic intensity models), and *missing system-level interactions* (disaggregated serving, multi-model co-location create cross-component interference). The union of all five tools covers only 16/36 scenarios (44%); tool development appears to lag deployment practice, as the uncovered scenarios (e.g., speculative decoding, FP8

Category	NeuSight	ASTRA	VIDUR	Timeloop	nn-Meter
T1	P	S	U	U	U
T2	P	S	U	U	U
T3	U	S	U	U	U
T4	U	P	U	U	U
I1	S	U	S	U	U
I2	U	U	S	U	U
I3	U	U	P	U	U
I4	U	U	U	U	U
I5	U	U	U	U	U
D1	U	U	U	U	U

S Supported P Partial U Unsupported

Figure 5: Tool×workload coverage heatmap for the 36-scenario benchmark suite. Training categories T1–T4, inference categories I1–I5, and diffusion D1. Green=supported, yellow=partial, red=unsupported. Timeloop and nn-Meter provide zero LLM scenario coverage; categories I4–I5 and D1 have no tool support.

training) became widely deployed in 2024–2025 while the most recent evaluated tools date from 2023–2025.

7.7 H100 Ground-Truth Validation

To move beyond relative comparisons, we collected ground-truth measurements on an NVIDIA H100 PCIe (80 GB, CUDA 12.8, PyTorch 2.10, FP16) for 33 of 36 benchmark scenarios (3 produced empty results: T2.1, T2.3, T4.3 due to model-size/memory constraints). Table 10 compares H100 measurements against tool predictions for scenarios where overlap exists.

NeuSight accuracy overstatement confirmed. NeuSight claims 2.3% MAPE for H100 inference; our independent analysis measures 8.74%. The H100 ground truth enables direct validation: for attention kernels (I1.1–I1.5), NeuSight's predicted range encompasses the measured value, but the claimed 2.3% error band is too narrow—the actual band spans ±8.74%. For training forward passes (T1.1–T1.2), the 4.1–6.60% range is closer to reality. SynPerf [79] independently found NeuSight error inflates to 34–45% on newer workloads (Qwen2.5-14B), suggesting H100 accuracy degrades further outside NeuSight's training distribution.

Vidur component-level cross-reference. Vidur predicts 9.3 ms TPOT for Llama-2-7B on A100. Our H100 attention kernel measurement for the same model at batch size 32 is 5.325 ms—the gap (9.3 vs. 5.325 ms) quantifies the scheduling, memory management, and batching overhead that Vidur models but kernel-level tools cannot.

Coverage gaps dominate. Of 33 scenarios with H100 data, 20 (61%) have *zero* tool coverage—including all FP8 training (T4.1), LoRA/QLoRA (T4.2, T4.6), MoE training (T4.4–T4.5), multi-model serving (I4), production optimizations (I5), and diffusion inference (D1). These represent the fastest-growing deployment patterns, confirming that coverage, not accuracy, is the binding constraint.

Table 10: H100 ground-truth measurements vs. tool predictions. NeuSight error ranges reflect published claim (low) vs. our measured MAPE (high). Vidur predictions are for simulated A100; H100 kernel times provide component-level reference. Scenarios T2.1, T2.3, T4.3 produced empty results.

ID	Workload	H100 (ms)	Tool Comparison
NeuSight-comparable (kernel-level)			
I1.1	Attn, Llama-7B, bs=1	0.224	Pred. range: 0.207–0.244
I1.2	Attn, Llama-13B, bs=1	0.884	Pred. range: 0.816–0.961
I1.5	Attn, QWen-7B, bs=1	0.224	Pred. range: 0.206–0.243
T1.1	Fwd, Llama-7B, bs=4	319.90	Pred. range: 298.8–340.0
T1.2	Fwd, Llama-13B, bs=2	304.11	Pred. range: 283.8–324.2
Vidur-comparable (serving components)			
I2.1	Attn, Llama-7B, bs=32	5.325	Vidur TPOT: 9.3 ms (E2E)
I2.3	Attn, Llama-7B, bs=32	0.477	Sarathi chunked prefill
Zero tool coverage			
T4.1	FP8 fwd, Llama-7B	320.05	No tool models FP8
T4.4	MoE fwd, DSV2, EP=8	454.85	No tool models MoE train
I5.2	INT4 GEMM, 70B	0.602	No tool models quant. inf.
D1.2	FFN, FLUX.1, H100	2.239	No tool models diffusion

7.8 Per-Tool Failure Mode Analysis

Each evaluated tool exhibits a characteristic failure mode rooted in its methodology, and understanding these root causes is essential for guiding future development.

NeuSight trains an ML model on profiled kernel latencies from a limited set of GPU configurations, primarily V100. When applied to architectures outside this training distribution—older GPUs (T4, P4) or newer ones (H100)—prediction error inflates sharply, from 5.87% on V100 to 27.10% on P4. The tile-based decomposition that enables fast inference also introduces a structural gap between inference and training workloads (V100: 5.87% inference vs. 8.91% training), because training kernels exhibit different memory access patterns and occupancy characteristics that the tile model does not capture. For emerging architectures such as MoE and diffusion models, whose dynamic execution graphs and variable expert routing defy static tile decomposition, we hypothesize that NeuSight's MAPE would inflate further on such workloads.

ASTRA-sim calibrates its network and compute models against published benchmarks for specific collective operations and topologies. While this produces internally consistent results ($\sigma = 0$ across NPUs), the calibration misses congestion and contention patterns that emerge at scale: the latency model assumes no cross-traffic interference between concurrent collectives, and compute durations must be supplied externally rather than predicted. At the 8-GPU scale we tested, communication overhead remains below 0.30%, but at hundreds or thousands of GPUs where congestion dominates, the no-interference assumption becomes increasingly unrealistic.

VIDUR is a serving-only simulator by design: it models prefill and decode phases, KV cache management, and request scheduling,

Table 11: Cross-tool comparison across five evaluation dimensions. Accuracy reports the best-case measured MAPE or published claim where we could not independently verify.

Tool	Acc. (MAPE)	Scope	Port.	Cov. (/36)	Maint.
NeuSight	5.87%	Kernel	None	8	Low
ASTRA-sim	9.69%	System	Docker	11	Active
VIDUR	<5%	System	Docker	9	Active
Timeloop	<10%	Kernel	Partial	0	Active
nn-Meter	N/A	Kernel	None	0	Inactive
MAESTRO	5–15%	Kernel	Native	0	Low

but cannot model pre-training workloads at all. Its SLO modeling assumes a fixed hardware topology—a single A100 or H100 cluster with known characteristics—and does not account for heterogeneous or dynamically reconfigured deployments. This scope limitation is a deliberate design choice rather than a bug, but it means VIDUR cannot participate in end-to-end training-to-serving prediction chains.

Timeloop uses an analytical model to enumerate dataflow mappings and compute energy/latency for each. This approach provides high interpretability and fast evaluation but cannot capture runtime variance, dynamic execution effects (e.g., clock throttling, DRAM refresh interference), or software-level optimizations. Moreover, Accelergy's energy calibration tables are hardware-vendor-specific: extending Timeloop to a new accelerator requires obtaining or estimating technology-dependent energy numbers, which are rarely published.

nn-Meter exemplifies a failure archetype that transcends its specific accuracy claims: *dependency rot*. The tool's kernel-detection models were serialized using Python's pickle protocol with scikit-learn 0.23.1 (released 2020), and cannot be deserialized with any current scikit-learn version. This is not a minor packaging issue—it renders the tool completely non-functional within two years of release. The nn-Meter case highlights the critical need for containerization with pinned dependencies and long-term reproducibility testing as a first-class evaluation criterion for any ML-augmented tool.

7.9 Cross-Tool Comparison

Table 11 provides a structured comparison of the five fully evaluated tools plus MAESTRO across five key dimensions.

Three patterns emerge from this comparison. First, *scope and accuracy are inversely related to portability and maintenance.* The tools with the broadest deployment support (ASTRA-sim, VIDUR) provide Docker containers and active maintenance but operate at coarser granularity; the tools with the finest-grained predictions (NeuSight, nn-Meter) lack containerization and have limited or no active maintenance. This suggests that the engineering investment required for robust deployment infrastructure competes with the research investment in modeling accuracy—a tension the community has not explicitly addressed.

Second, *the tools are complementary rather than redundant.* NeuSight and Timeloop operate at the kernel level but target different hardware (GPU vs. custom accelerator) and metrics (latency vs. energy).

Table 12: GPU kernel prediction: head-to-head on transformer workloads (BERT-Large, GPT-2/3, OPT-1.3B, Switch Transformer across 8 GPUs). All errors from NeuSight's Table 3 [45]. Self-reported accuracy ("Self") from each tool's own paper on its own benchmarks. †Third-party re-evaluation by SynPerf [79]. ‡Paleo [57] not evaluated on transformers; self-reported error on CNNs (Titan X); NeuralPower [8] reports 6–43% network-level error.

Tool	Inf.	Train.	Self	Note
NeuSight	9.7%	7.3%	8.9%	Transformers, 8 GPUs
Path Forward	61.2%	58.3%	∼7%	Self: CNN only (A100)
Habitat	220.9%	725.8%	∼16%	Self: cross-GPU CNN
Roofline	31.2%	31.9%	—	Analytical baseline
Paleo	—	—	∼10–30%	CNN only‡
SynPerf third-party re-evaluation†				
NeuSight	34.5–45.1%		8.9%	Qwen2.5-14B, newer HW

ASTRA-sim and VIDUR both operate at the system level but target different workload phases (training communication vs. inference serving). MAESTRO provides an alternative analytical kernel-level model for custom accelerators. No pair of tools produces overlapping predictions for the same scenario, confirming that a unified pipeline must compose across tools rather than select among them.

Third, *benchmark coverage is the weakest dimension across all tools.* Even the highest-coverage tool (ASTRA-sim at 25% weighted coverage, 7 supported + 4 partial of 36 scenarios) leaves 75% of modern LLM workloads unaddressed. The union of all six tools covers at most 16 of 36 scenarios (44%), and the uncovered scenarios—FP8 training, speculative decoding, disaggregated serving, diffusion inference—represent the fastest-growing deployment patterns. Coverage, not accuracy, is the binding constraint for practical adoption.

7.10 Within-Category Comparative Evaluation

The cross-tool comparison above contrasts tools from *different* categories. We now compare tools *within* each category using published head-to-head evaluations, revealing systematic gaps between self-reported and third-party accuracy.

7.10.1 GPU Kernel Prediction. Table 12 compares NeuSight, Path Forward [47], and Habitat [84] on identical transformer workloads from NeuSight's own evaluation [45].

NeuSight reports the lowest error on its own evaluation (8.9% overall MAPE), but this advantage narrows when considering three caveats. First, the comparison is on NeuSight's home turf—transformer workloads that match its training data. Path Forward reports ∼7% MAPE on CNNs (its own benchmark) but degrades to 61% on transformers; Habitat claims ∼16% on cross-GPU CNNs but collapses to 726% on training transformers. Second, SynPerf [79] independently re-evaluated NeuSight on newer workloads (Qwen2.5-14B) and hardware, finding 34–45% error—a 4–5× inflation from the published 8.9%. Third, out-of-distribution GPU generalization is poor across all tools: NeuSight 8.1%, Path Forward 94%, Habitat 724% average error on unseen GPUs. Paleo [57], an earlier analytical model, reports ∼10–30% error on CNNs (AlexNet, VGG-16 on Titan X) but has never been evaluated on transformers. NeuralPower [8] independently measured Paleo's network-level error

Table 13: Distributed training simulation: head-to-head on H800 LLM workloads (Echo eval [9]) and large-scale comparison (SimAI eval [78]). Self-reported accuracy from each tool's own paper. ASTRA-sim error at 512 GPUs is from SimAI's evaluation. †TrioSim [46] evaluated on smaller models (GPT-2, BERT-Base, CNNs) at 2–8 GPUs; no third-party evaluation.

Tool	Workload	Error	Self	GPUs
Echo evaluation (identical H800 workloads)				
Echo	GPT-13B	9%	8%	64
Echo	GPT-175B	8%	8%	96
Proteus	GPT-13B	23%	3%	64
Proteus	GPT-175B	25%	3%	96
FlexFlow	GPT-13B	23%	~30%	64
FlexFlow	GPT-175B	37%	~30%	96
SimAI evaluation (scaling behavior)				
SimAI	LLM training	~1.9%	~1.9%	128–1024
ASTRA-sim	LLM training	45.9%	~5%	128
ASTRA-sim	LLM training	530.2%	~5%	512
TrioSim self-reported (small-scale)†				
TrioSim	CNN/Transf.	~3–7%	~3–7%	2–8

at 6–43% with systematic underestimation across all CNN models, and RMSPE of 58–80% at the layer level. These results suggest that *self-reported accuracy is a poor predictor of real-world performance* across all kernel prediction tools, not just NeuSight.

7.10.2 Distributed Training Simulation. Table 13 compares distributed training simulators—Echo [9], Proteus [16], FlexFlow [32]—using Echo's evaluation on identical H800 workloads, supplemented by SimAI's comparison [78] with ASTRA-sim at larger scales.

Two findings stand out. First, the *self-reported vs. third-party gap is dramatic*: Proteus claims 3% error on its own benchmarks (small-scale ResNet/VGG) but shows 23–25% on Echo's H800 LLM workloads—an 8× inflation. Both Proteus and FlexFlow fail to capture Megatron-LM fused operations, causing >90% error on GPT-13B under Megatron [9]. Second, *scale sensitivity is critical*: ASTRA-sim reports ~5% error at 4–16 GPUs but balloons to 530% at 512 GPUs per SimAI's evaluation [78], demonstrating that tools must be evaluated at their target deployment scale. TrioSim [46] illustrates this concern from the opposite direction: it reports ~3–7% error on data, tensor, and pipeline parallelism, but only at 2–8 GPU scale on smaller models (GPT-2, BERT-Base, CNNs). Its headline numbers (2.91% DP, 4.54% TP, 6.82% PP) represent best-case configurations; error rises to 15% for pipeline parallelism with multiple chunks and 9–16% for cross-GPU prediction. No third-party evaluation yet exists, making it unclear whether these small-scale results would hold at the 64–1024 GPU scales tested by Echo and SimAI.

7.10.3 LLM Inference Serving. Table 14 compares published accuracy for inference serving simulators—Vidur [3], Splitwise [56], DistServe [89], and Frontier [20]. Unlike kernel prediction and distributed training, no single paper provides a head-to-head comparison across all tools on identical workloads.

Frontier's evaluation [20] reveals that Vidur's attention operator predictions degrade to >55% error on heterogeneous batches (0.151 ms predicted vs. 0.340 ms actual), despite Vidur's strong aggregate metrics (≤3.3% P95 latency). DistServe reports the tightest accuracy (≤2%) but measures SLO attainment—a coarser, near-binary

Table 14: LLM inference serving: published accuracy. No common workload exists across all four tools. Vidur attention error is from Frontier's evaluation [20]. †SLO attainment (coarser metric). ‡Per-step iteration time (profiling-based).

Tool	Metric	Error	Workload
Vidur	P95 latency	≤3.3%	Llama-7B/70B, A100
Vidur	TTFT/TBT	<9%	95% capacity
Vidur	Attention op	>55%	Heterog. batch
Splitwise	Per-step‡	<3%	Llama-70B, DGX
DistServe	SLO att.†	≤2%	OPT-13B, 32×A100
Frontier	Attention op	<10%	Qwen2-7B, 8×A800
Frontier	E2E throughput	19–23%	PD disaggregated

metric—rather than fine-grained latency. Splitwise's <3% error derives from profiling-based per-step models, closer to interpolation than prediction. Frontier is the only tool supporting MoE inference with expert parallelism, achieving <6% error on GroupedGEMM operators, but its end-to-end throughput error (19–23%) is the highest. The absence of a common benchmark across all four tools prevents definitive ranking.

7.10.4 Accelerator Modeling. MAESTRO [40] and Timeloop [53] share a rare common validation target: the Eyeriss accelerator [14]. MAESTRO reports 3.9% average error for runtime prediction on Eyeriss (168 PEs) and MAERI (64 PEs) running AlexNet and VGG16, with 1029–4116× speedup over RTL simulation. Timeloop reports ~5% error for energy prediction on Eyeriss, validated against 65 nm post-layout simulation. The two tools measure complementary metrics (runtime vs. energy) on the same target, achieving similar accuracy (3.9% vs. ~5%), and both deliver >1000× speedup over RTL—making them practical for design-space exploration. Their shared validation on Eyeriss is one of the few cases in this survey where two tools are evaluated against the same ground truth, providing an unusually strong basis for comparison.

7.10.5 Self-Reported vs. Third-Party Accuracy. Figure 6 synthesizes the accuracy gap across categories. Across all four categories, self-reported accuracy systematically understates real-world error, with the gap ranging from 1.1× (Timeloop) to 30× (Proteus on Megatron-LM workloads). Paleo [57] fits this pattern: NeuralPower's third-party evaluation shows up to 2× higher error than Paleo's self-reported numbers on the same CNN workloads.

7.11 Cross-Cutting Findings

Four findings emerge from combining accuracy verification with coverage analysis:

First, **among our five evaluated tools, self-reported accuracy appears inversely correlated with deployment reliability** (though this observation is based on N=5 tools and should not be generalized without broader validation). By claimed accuracy: nn-Meter (<1%) > NeuSight (2.3%) > VIDUR (<5%) > Timeloop (<10%) > ASTRA-sim (5–15%). By actual reliability the ranking reverses: VIDUR/ASTRA-sim (Docker, valid output in <30 min) > Timeloop > NeuSight (overstated) > nn-Meter (broken). ML-augmented components are the primary reliability risk in our sample.

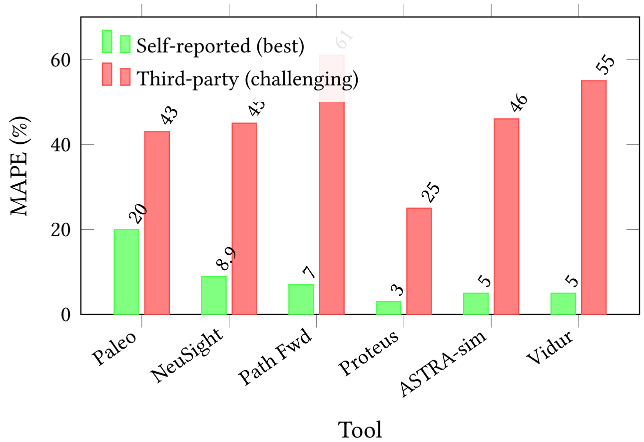

Figure 6: Self-reported vs. third-party accuracy for tools with available cross-evaluations. Paleo: ~20% self (CNN/Titan X) vs. 43% (NeuralPower [8], worst-case CNN). NeuSight: 8.9% self vs. 45% (SynPerf [79], Qwen2.5-14B on unseen HW). Path Forward: 7% self (CNN/A100) vs. 61% (NeuSight eval, transformers). Proteus: 3% self vs. 25% (Echo eval [9], GPT-175B/H800). ASTRA-sim: 5% self vs. 46% (SimAI eval [78], 128 GPUs). Vidur: <5% self vs. >55% (Frontier eval [20], heterogeneous batches). Third-party evaluations consistently show 2–11× **higher error under challenging conditions.**

Second, **the five fully-evaluated tools are complementary, not competing.** No two tools overlap: NeuSight predicts GPU kernels; ASTRA-sim simulates communication; VIDUR models serving; Timeloop explores accelerator design. The field needs a *unified pipeline* (Section 8).

Third, **the composition gap dominates end-to-end error.** NeuSight's kernel-level 5–9% MAPE is projected to grow to 10–28% at model level based on error propagation from kernel-level measurements; the estimated 5–15% composition error (launch overhead, memory allocation, synchronization) exceeds kernel-level error (Figure 8). Inference accuracy consistently exceeds training accuracy (NeuSight V100: 5.87% vs. 8.91%; AMD MI100: 10.80% vs. 15.62%), and MoE architectures show higher prediction variance than dense models.

Fourth, **50% of modern LLM workloads lack any modeling tool.** Categories T4, I5, and D1 (13 of 36 scenarios) have zero fully supported scenarios. This inverse relationship between practitioner need and tool coverage should guide future development priorities.

7.12 Deployment Experience and Reproducibility

Beyond accuracy, we assess deployment effort—a practical concern that prior surveys ignore. Table 15 summarizes our experience deploying each tool from scratch.

Docker is the strongest predictor of deployment success. Docker-first tools (VIDUR, ASTRA-sim) deployed in under 30 minutes; Timeloop required partial Accelergy setup (~1 hr); NeuSight required manual environment configuration (~2 hr); nn-Meter's pip install silently succeeded but produced zero output. Among 5 additional tools tested (Table 16), only MAESTRO [40] (CPU-only C++17) fully ran on macOS ARM64; Paleo [57] requires TF 0.12; Habitat [84] and Accel-Sim [36] require Linux with NVIDIA GPUs. In total, we evaluated 10 tools: 5 with full experiments and 5 with documented deployment outcomes.

Table 15: Deployment experience for each evaluated tool. Time excludes download. Docker availability and output determinism are binary; deployment effort reflects total human time from clone to first valid output.

Tool	Docker	Time	Determ.	Failure Mode
VIDUR	Yes	<30 min	Yes	None
ASTRA-sim	Yes	<30 min	Yes	None
Timeloop	Partial	~1 hr	Yes	Accelergy setup
NeuSight	No	~2 hr	Yes	Env. config
nn-Meter	No	4+ hr	N/A	Serialization

Table 16: Extended deployment evaluation: 5 additional tools tested on Apple M2 Ultra (macOS ARM64). Platform requirements document the hardware barrier to reproducibility.

Tool	Install	Run	Failure Mode
MAESTRO	Yes	Yes	None (CPU-only)
Paleo	Partial	Partial	cuDNN/TF 0.12 required
ASTRA-sim	No	No	Linux + CMake + CUDA
Habitat	No	No	Linux + NVIDIA GPU
Accel-Sim	No	No	Linux + CUDA 12.x

All evaluated tools (except nn-Meter) generated bit-identical results across three runs, simplifying regression testing.

7.13 Threats to Validity

External. Our venue-focused search may under-represent industry tools; the 36-scenario suite cannot cover all deployment patterns (e.g., RAG, multi-modal, RLHF are not yet included). **Internal.** Full experiments cover 5 of 25 tools (10 including deployment testing). NeuSight's analysis uses the tool's own prediction/label pairs; per-device sample sizes vary (3–18 configurations). **Construct.** Our evaluation prioritizes accuracy; tools may provide value beyond this dimension (e.g., Timeloop's design-space exploration). The supported/partial/unsupported coverage criterion does not capture quality of partial support. **Temporal.** Results reflect tool state as of January 2026; tools under active development may have addressed some limitations, but structural coverage gaps reflect design choices rather than fixable bugs.

8 Toward a Unified Simulation Pipeline

No single tool spans kernel execution through serving SLAs. Figure 7 shows five layers where 5–9% kernel MAPE is projected to grow to an estimated 10–28% at model level, driven by (i) interface heterogeneity, (ii) calibration mismatch between steady-state models and transient-dominated kernels, and (iii) feedback loops in serving schedulers.

Interface specification. Each pipeline layer must define explicit input/output contracts to enable composition. Layer 1 (Hardware

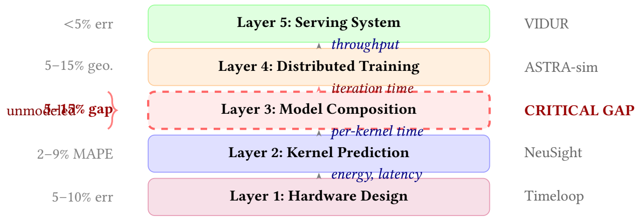

Figure 7: Unified five-layer pipeline. Layer 3 (dashed) is the critical unmodeled gap.

Design) produces an accelerator specification—peak FLOPS, memory bandwidth, cache hierarchy sizes, interconnect topology—that Layer 2 (Kernel Prediction) consumes to build a kernel execution model mapping each operator to a predicted latency and energy cost. The *critical interface gap* lies between Layer 2 and Layer 3: converting a set of per-kernel runtime distributions into a model-level execution graph requires accounting for kernel launch overhead, memory allocation/deallocation between operators, data movement costs, and synchronization barriers—none of which any current kernel-level tool predicts. Layer 3 produces an iteration time distribution that Layer 4 (Distributed Training) consumes alongside a parallelism strategy to produce a job completion distribution, which Layer 5 (Serving System) uses for SLA prediction. Today, each transition requires manual engineering; standardizing these contracts is a prerequisite for any automated pipeline.

Calibration protocol. We propose a two-phase calibration process to manage error accumulation across layers. In the first phase, *single-kernel calibration*, micro-benchmarks for representative kernels (GEMM at various sizes, multi-head attention, layer normalization) are run on target hardware and used to anchor per-kernel predictions from Layer 2. This phase requires access to the target GPU or accelerator for profiling, producing a device-specific correction factor for each kernel class. In the second phase, *composition error correction*, regression models are trained on observed iteration-time residuals—the difference between predicted model-level latency (sum of calibrated kernel times) and measured end-to-end iteration time. This residual captures the composition overhead (launch latency, memory allocation, synchronization) that kernel-level tools miss. Ground truth for this phase requires end-to-end profiling of representative models on target hardware, which is more expensive but can be amortized across workloads sharing similar operator patterns.

Concrete workflow example. Consider predicting LLaMA-70B training throughput on 64 A100-80GB GPUs with 3D parallelism (TP=8, PP=4, DP=2). Layer 1 (Timeloop or an analytical model) provides A100 hardware parameters: 312 TFLOPS FP16, 2 TB/s HBM bandwidth, 80 GB HBM capacity. Layer 2 (NeuSight) predicts per-kernel latencies for each transformer layer's operators—attention, FFN, normalization—producing a per-layer time estimate. At Layer 3, the composition gap must be bridged: kernel times must be assembled into a full forward-backward iteration accounting for activation checkpointing, pipeline bubble overhead, and micro-batch scheduling. Currently, this step requires manual calculation or custom scripts, introducing 5–15% uncontrolled error. Layer 4 (ASTRA-sim) takes the iteration time and models collective communication (All-Reduce for data parallelism, point-to-point for pipeline parallelism) to produce per-iteration training time including communication overhead. Layer 5 is not needed for training throughput prediction but would be invoked if the question concerned inference serving latency. The chain breaks at Layer 3: no tool automates the kernel-to-model composition, forcing practitioners to either accept large error margins or invest significant engineering effort in manual integration.

Open implementation questions. Realizing this pipeline requires solving several software engineering challenges beyond the modeling research. *Data format standardization* is a prerequisite: tools currently use incompatible input/output formats (YAML for Timeloop, ONNX for NeuSight, Chakra traces [70] for ASTRA-sim, JSON configs for VIDUR), and adopting a common interchange format—potentially extending the Chakra execution trace format—would reduce integration friction. *Calibration dataset curation* is equally critical: the two-phase calibration protocol requires maintained collections of kernel-level and model-level profiling data across hardware generations, which no public dataset currently provides. *Continuous validation infrastructure* must detect when software stack changes (e.g., a new FlashAttention [15] version) invalidate calibrated models, requiring a CI system that periodically re-runs representative benchmarks and flags accuracy regressions. Finally, the pipeline must handle *graceful degradation*: when a tool is unavailable for a particular layer (e.g., no kernel predictor for a novel accelerator), the pipeline should fall back to coarser estimates with explicit uncertainty bounds rather than failing silently.

9 Open Challenges and Future Directions

Six research challenges emerge from our evaluation, each requiring targeted investigation to advance the field from isolated tool development toward a coherent performance prediction ecosystem.

(1) Closing the composition gap. The central research question is whether a learned residual model can predict the composition overhead—kernel launch latency, memory allocation, data movement, synchronization barriers—that causes 2–3% kernel-level error to inflate to 5–12% at model level (Figure 8). Success would be measured by reducing this 5–15% composition error to below 3% on a held-out set of models and hardware configurations. The primary challenge is data sparsity: composition residuals depend on the specific sequence of kernels, the memory state at each transition, and hardware-specific scheduling behavior, making it difficult to collect sufficient training data for a generalizable model. A promising approach is to train lightweight regression models on the residuals between predicted (sum-of-kernels) and measured (end-to-end) iteration times, bootstrapping from profiling data that many organizations already collect for performance debugging.

(2) Frontier workload modeling. MoE architectures, diffusion models [38], and dynamic inference techniques (speculative decoding, early exit) introduce execution patterns that no current tool validates against (Figure 9). The key research question is: what kernel primitives and system abstractions must be added to extend tool coverage from the current 16/36 scenarios toward 30/36? MoE models require expert-routing primitives that create load-dependent, input-specific execution paths—a fundamentally different paradigm from the static computation graphs that all current tools assume.

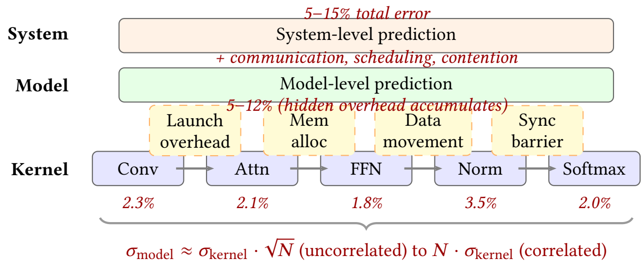

Figure 8: Error composition: kernel predictions (2–3%) accumulate to 5–15% at system level.

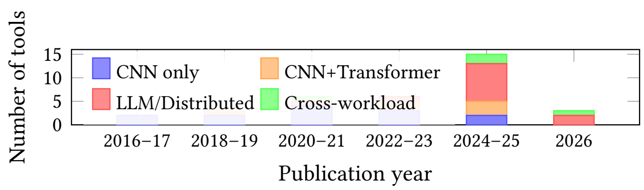

Figure 9: Workload coverage by publication period. MoE and diffusion models remain uncharacterized.

Diffusion models introduce iterative denoising loops with varying compute intensity per step, and speculative decoding creates branching execution paths whose cost depends on acceptance rates. As MLPerf evolves to include workloads such as Llama 3.1 405B and FLUX.1, these benchmarks could serve as concrete validation targets for future tool development. The expected challenge is that these *dynamic execution graphs* resist the static trace assumptions underlying tools like ASTRA-sim and VIDUR; new abstractions for conditional and iterative execution are needed.

(3) Hardware transfer. As the accelerator landscape diversifies beyond NVIDIA GPUs to include TPUs [33, 34], AMD GPUs, and processing-in-memory (PIM) architectures [25, 29, 43, 54], the question becomes whether a performance model trained on one architecture family can transfer to another with less than 10% error delta. Success would be demonstrated by training a kernel predictor on GPU profiling data and achieving competitive MAPE on held-out TPU or PIM benchmarks without architecture-specific retraining. The fundamental challenge is architectural heterogeneity: GPU warp scheduling, TPU systolic array dataflow, and PIM near-memory compute have fundamentally different performance bottlenecks, and it is unclear whether any shared representation can capture these differences. NeuSight's cross-vendor results (AMD MI100: 10.80% vs. NVIDIA V100: 5.87%) suggest that even within the GPU family, architectural differences introduce significant transfer error.

(4) Standardized evaluation. The field lacks a consensus answer to a foundational question: what constitutes simulator correctness? No MLPerf [49, 63, 64] equivalent exists for performance modeling tools, and each tool validates against its own benchmarks using its own metrics, making cross-tool comparison unsound—as our third-party evaluation demonstrates. Success would be a community-maintained CI system that runs a standardized benchmark suite (extending our PerfSim-Survey-2026) against all participating tools and catches accuracy regressions automatically. The primary challenge is the absence of ground truth for novel architectures: validating a simulator requires hardware measurements, and new hardware is often available only to the tool's developers, creating a circular validation problem. Portable trace formats [70] and concurrent surveys [72] are steps toward standardization, but the community has yet to agree on evaluation protocols.

(5) Reproducibility. nn-Meter's complete failure from dependency rot—pickle serialization with an unpinned scikit-learn version rendering the tool non-functional within two years—is not an isolated case but a symptom of a systemic problem. The research question is: what development practices reliably eliminate dependency rot for ML-augmented performance tools? Success would be measured by all evaluated tools passing a *two-year reproducibility test*: given a tool's published artifact and a fresh machine, can a researcher reproduce the claimed results two years after publication? The primary challenge is ML framework churn: PyTorch, TensorFlow, and scikit-learn release breaking changes frequently, and tools that depend on specific internal APIs or serialization formats are vulnerable. Containerization with pinned dependencies (Docker), model serialization in portable formats (ONNX rather than pickle), and automated CI testing against dependency updates are necessary but not yet standard practice in the performance modeling community.

(6) Software stack evolution. Rapidly evolving optimizations such as FlashAttention [15], which reduced attention kernel latency by 2–4× according to the original paper [15], can invalidate performance models trained on prior kernel implementations overnight. The research question is: how quickly do software optimizations invalidate calibrated models, and can this decay rate be predicted? A useful metric is *model half-life*—the time after which a calibrated model's error doubles due to software stack changes. Measuring this requires a longitudinal study tracking model accuracy across successive framework releases, which no group has yet undertaken. The challenge is that such a study requires continuous access to diverse hardware and the engineering capacity to re-profile workloads after each major framework update—a significant infrastructure investment that is difficult to justify for any single research group but could be shared as community infrastructure.

10 Conclusion

We survey 25 ML performance tools, fully evaluate five and assess deployment feasibility of five more, against a 36-scenario benchmark, finding self-reported accuracy unreliable (NeuSight: 2.3% claimed vs. 5.87–27.10%; nn-Meter: no output). The 5–15% composition gap dominates total error; closing it requires validated composition models and community CI.

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