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

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Anonymous Author(s)
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Anonymous

Abstract

As machine learning workloads grow in scale and complexity, architects need fast, accurate methods to predict performance across diverse hardware. This survey analyzes 22 tools from 53 papers across architecture and systems venues (2016–2026), covering analytical models, trace-driven simulators, and ML-augmented hybrid techniques for DNN accelerators, GPUs, distributed training, and LLM inference serving. We organize the literature by methodology type, target platform, and abstraction level, revealing a pervasive CNN-validation bias and finding that hybrid approaches achieve the best accuracy-speed trade-offs. We conduct hands-on evaluations of representative tools, independently measuring their performance and accuracy rather than relying on original claims; tools with Docker-first deployment remain reproducible, while those relying on serialized ML models become unusable. We identify open challenges including cross-workload generalization, kernel-to-end-to-end error composition, and emerging architecture support, providing practitioners tool selection guidance and researchers a roadmap for the field.

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 [33, 34] 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 [54], MAESTRO [42]) evaluate in microseconds with 5–15% error. Trace-driven simulators (ASTRA-sim [78], VIDUR [3]) replay execution traces for system-level modeling. Hybrid approaches (NeuSight [46]) combine analytical structure with learned components to achieve 2.3% error. Yet no comprehensive survey organizes these methods for the practitioner who must select a tool for a specific task. Existing surveys focus on ML *techniques* for modeling [71] or specific hardware [54]; this survey fills that gap with a methodology-centric view.

We make the following contributions:

- A **methodology-centric taxonomy** organizing tools along three dimensions: methodology type, target platform, and abstraction level, with a coverage matrix identifying research gaps and a workload analysis exposing CNN-validation bias.
- A **systematic survey** of 22 tools from 53 papers across architecture venues (MICRO, ISCA, HPCA, ASPLOS) and systems venues (MLSys, OSDI, NSDI) published 2016–2026.
- A **comparative analysis** of accuracy–speed trade-offs with careful qualification of reported claims.
- **Hands-on evaluations** where we independently measure tool performance and accuracy, and identification of **open challenges** including the CNN-to-transformer generalization gap, kernel-to-end-to-end error composition, and emerging accelerator support.

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

2 Survey Methodology

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

Related surveys. Prior surveys address adjacent topics: Rakhshanfar and Zarandi [60] survey ML for processor DSE; Sze et al. [72] treat DNN hardware design (the foundation for Timeloop/MAESTRO); simulators such as GPGPU-Sim [4], gem5 [6], and SST [64] have been extensively used as validation targets in the performance

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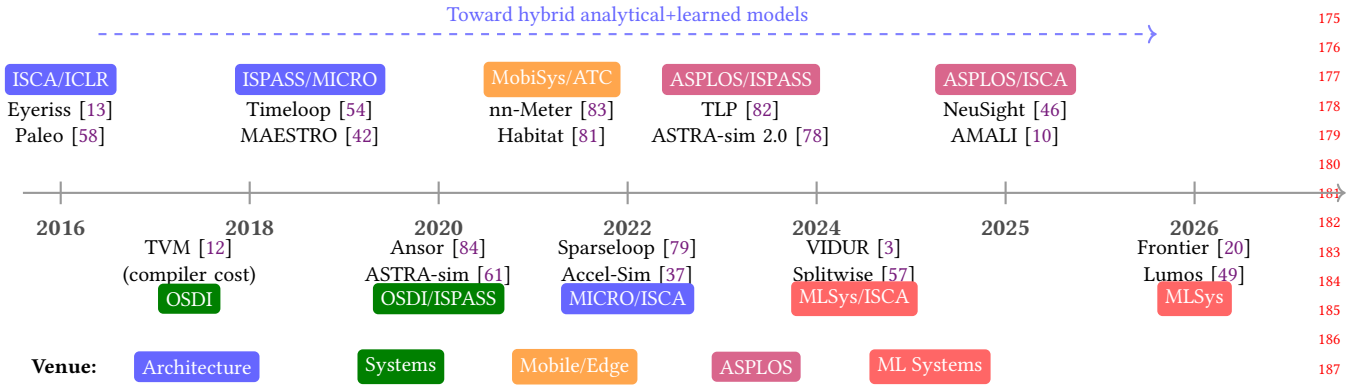

Figure 1: Evolution of performance modeling tools for ML workloads (2016–2026). Colors indicate publication venue category. Early analytical frameworks (Eyeriss, Paleo) gave way to systematic accelerator modeling (Timeloop, MAESTRO) and distributed training simulation (ASTRA-sim). Recent work targets LLM-specific modeling (VIDUR, Frontier) and hybrid approaches (NeuSight).

modeling literature; and MLPerf [51, 63] standardizes *measurement* rather than *prediction*. Early ML accelerator modeling (2014–2018) established foundational approaches: DianNao [11] introduced analytical dataflow modeling for dedicated accelerators, Eyeriss [13] systematized row-stationary dataflow analysis, and Paleo [58] pioneered layer-wise analytical estimation. This survey differs by spanning the full methodology spectrum across all major platforms with hands-on evaluations. The closest prior work, Dudziak et al. [17], compares edge device predictors for NAS; we broaden to the full landscape.

3 Background

3.1 ML Workload Characteristics

ML workloads are expressed as computation graphs whose operator shapes are statically known and amenable to analytical modeling. Frameworks such as PyTorch [56] and TensorFlow [1] compile these graphs for execution, though MoE and dynamic inference introduce input-dependent control flow. Performance depends on tensor-to-memory mapping (dataflow, tiling), KV cache management for LLM inference [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 [57], both modeled under batched serving [2, 80].

3.2 Modeling Methodologies

We classify approaches into five categories. **Analytical models** express performance as closed-form functions (e.g., the roofline model [77]), offering microsecond evaluation but requiring per-architecture derivation. **Cycle-accurate simulators** (GPGPU-Sim [4], Accel-Sim [37]) achieve high fidelity at 1000–10000× slowdown, serving primarily as validation oracles for the high-level methods that are the focus of this survey. **Trace-driven simulators** (ASTRA-sim [78], VIDUR [3]) trade fidelity for orders-of-magnitude speedup. **ML-augmented approaches** learn from profiling data (nn-Meter [83]) but may not generalize beyond training distributions. **Hybrid approaches** combine analytical structure with learned components (NeuSight [46], Habitat [81]), aiming to balance accuracy, speed, and interpretability.

3.3 Problem Formulation

Performance modeling predicts a target metric (latency, throughput, energy, or memory footprint) given a workload description and hardware configuration. Workloads are represented at the operator, graph, IR, or trace level; hardware is characterized by specifications, performance counters, or learned embeddings. Ground-truth measurements typically rely on hardware performance counters accessed via PAPI [7] or LIKWID [73]. Accuracy metrics—MAPE, RMSE, and rank correlation—vary across the literature, and differences in benchmarks, hardware targets, and evaluation protocols limit direct comparison (Section 6).

4 Taxonomy

We organize the literature along three dimensions. The *primary axis* is methodology type—how a tool predicts performance—because methodology determines the fundamental trade-offs between accuracy, speed, interpretability, and data requirements. The *secondary axes* are target platform and abstraction level, which together determine the scope and applicability of each tool. We additionally characterize tools by workload coverage, exposing a pervasive CNN-validation bias in the literature.

Table 1 provides a unified view combining the coverage matrix (number of surveyed tools per methodology–platform cell) with trade-off profiles, with empty cells highlighting research gaps. 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.

Table 1 reveals three structural gaps: (1) trace-driven *execution replay* simulation (as distinct from instruction-trace-driven cycle-accurate simulation such as Accel-Sim) is used exclusively for distributed systems; (2) edge devices are served only by ML-augmented approaches, lacking hybrid alternatives; (3) no ML-augmented tool

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

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

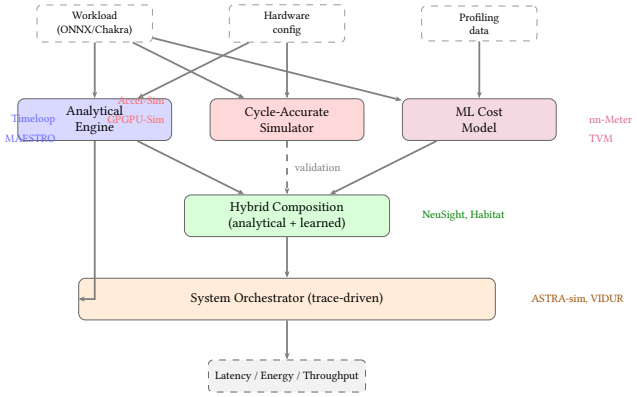

Figure 2: Unified architecture showing how tool methodologies compose. Analytical engines and ML cost models feed into hybrid approaches, while system-level orchestrators (trace-driven) assemble component predictions into end-to-end estimates. Cycle-accurate simulators primarily serve as validation oracles.

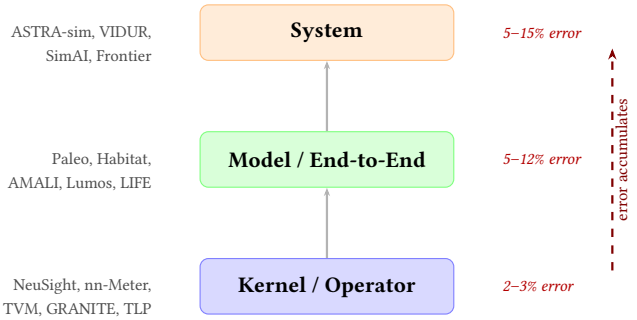

Figure 3: Abstraction level hierarchy and the composition problem. Tools operate at one of three levels; composing predictions across levels accumulates error. Error ranges are representative values from surveyed papers.

targets distributed systems directly. Methodologies cluster into two speed regimes: sub-millisecond (analytical, ML-augmented, hybrid) for DSE, and minutes-to-hours (simulation, trace-driven) for validation.

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

4.1 Primary Axis: Methodology Type

The choice of methodology determines fundamental trade-offs between accuracy, evaluation speed, data requirements, and interpretability, as summarized in Table 1; Section 5 provides detailed per-tool analysis.

Analytical models (Timeloop [54]: 5–10% vs. RTL; MAESTRO [42]; Sparseloop [79]; AMALI [10]) provide microsecond evaluation and full interpretability but require per-architecture derivation (AMALI's 23.6% MAPE illustrates GPU dynamic effects). **Cycle-accurate simulators** (GPGPU-Sim [4], Accel-Sim [37]: 0.90–0.97 IPC; PyTorch-Sim [38]) are impractical for DSE at 1000–10000× slowdown [4, 37]. **Trace-driven simulators** (ASTRA-sim [78]: 5–15%; VIDUR [3]: <5%; SimAI [75]; Frontier [20]) replay execution traces for system-level modeling. **ML-augmented models** (nn-Meter [83]; LitePred [18]; HELP [45]; TVM [12]/Ansor [84]) learn from profiling data but risk *silent distribution shift*. **Hybrid** approaches (NeuSight [46]: 2.3% MAPE; Habitat [81]; ArchGym [41]) combine analytical priors with learned corrections [17].

4.2 Secondary Axes: Platform and Abstraction Level

Platform constrains methodology: **accelerators** use analytical models; **GPUs** span all types; **distributed systems** require trace-driven simulation; **edge devices** use ML-augmented approaches; **CPUs** [53, 71] are least studied. Abstraction level determines composition errors (Figure 3): kernel-level tools achieve 2–3% error, model-level 5–12%, and system-level 5–15%, with errors propagating through the chain.

4.3 Workload Coverage

Table 2 characterizes the workload types on which each tool has been validated, exposing a pervasive CNN-validation bias.

Figure 4 quantifies this CNN-validation bias: of the 14 surveyed tools, 9 (64%) include CNN validation, while only 1 tool validates on MoE workloads and none validates on diffusion models. The table reveals that **no surveyed tool has been validated on diffusion models or dynamic inference workloads** [39], only Frontier [20] has validated MoE support, and no single tool offers

Table 2: Workload validation coverage. ✓ = validated in the original paper; ○ = partial or indirect validation; — = no validation. Nearly all tools report accuracy on CNN workloads; transformer and MoE coverage is sparse. Empty columns (diffusion, dynamic inference) represent workload types with *no* validated performance modeling tools.

Tool	CNN	Trans-former	LLM Train	MoE	Diff.
Timeloop	✓	○	—	—	—
MAESTRO	✓	—	—	—	—
NeuSight	✓	✓	—	—	—
Habitat	✓	—	—	—	—
AMALI	—	✓	—	—	—
ASTRA-sim	✓	○	✓	—	—
VIDUR	—	✓	—	—	—
SimAI	—	—	✓	—	—
Lumos	—	—	✓	—	—
Frontier	—	✓	—	✓	—
nn-Meter	✓	—	—	—	—
LitePred	✓	—	—	—	—
HELP	✓	—	—	—	—
TVM/Ansor	✓	○	—	—	—

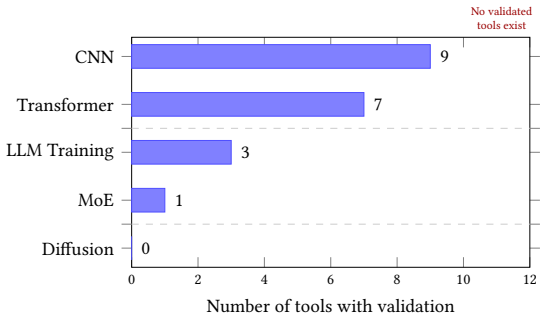

Figure 4: Workload validation coverage across surveyed tools. CNN validation dominates (64% of tools), while MoE and diffusion models have minimal or no validated prediction tools, highlighting a critical generalization gap.

validated transformer prediction across the full kernel-to-system stack. Practitioners working with non-CNN workloads must accept unvalidated predictions, collect their own validation data, or fall back to measurement.

5 Survey of Approaches

This section surveys performance modeling tools for ML workloads, organized by target platform, examining modeling challenges, available tools, and their strengths and limitations. Table 3 provides a comprehensive comparison.

5.1 DNN Accelerator Modeling

The analytical tractability of DNN accelerator modeling stems from the regularity of computation [72], building on early characterization pioneered by DianNao [11]. A convolution layer maps to a seven-deep nested loop over batch, output channel, input channel, and spatial dimensions; Timeloop [54] enumerates mappings of these loops to a spatial-temporal hardware hierarchy, computing data reuse at each memory level as the ratio of loop bounds. This exhaustive search finds the optimal dataflow in microseconds (5–10% error, 2000× speedup) because the search space, though combinatorially large, admits efficient pruning: any mapping that exceeds a memory level's capacity is immediately discarded. MAESTRO [42] achieves similar modeling with a more compact "data-centric" representation that specifies which data dimension is stationary at each level, trading enumeration completeness for specification simplicity—but sacrificing Timeloop's ability to model per-PE utilization, explaining why Timeloop achieves tighter error bounds on architectures with irregular PE arrays. SCALE-Sim [66] complements both by providing cycle-accurate systolic array simulation for validation. Sparseloop [79] extends Timeloop's analysis to sparse tensors by introducing format-specific access count models for compression formats (CSR, bitmap)—the key challenge being that sparse data access patterns depend on the data values, requiring statistical or format-aware modeling rather than purely geometric analysis. PyTorchSim [38] integrates PyTorch 2 with NPU simulation but lacks real-hardware validation; ArchGym [41] connects ML surrogates to simulators (0.61% RMSE vs. simulator, not hardware). Accelerator modeling is the most mature subdomain, with Timeloop as the de facto DSE standard. The key gap is silicon validation; emerging PIM tools [26, 31, 44, 55] also lack hardware validation.

5.2 GPU Performance Modeling

GPUs dominate ML training and inference, requiring models for SIMT execution, warp scheduling, memory coalescing, and occupancy effects.

Cycle-accurate simulation. GPGPU-Sim [4] and Accel-Sim [37] achieve 0.90–0.97 IPC correlation but at 1000–10000× slowdown; reverse-engineering [30] improved Accel-Sim to 13.98% MAPE. These simulators integrate with memory subsystem models—from DRAMSim2 [65] and Ramulator [40] to their modern successors DRAMSim3 [48] and Ramulator 2.0 [50]—for accurate DRAM timing, critical for memory-bound LLM inference.

Analytical and hybrid models. AMALI [10] models GPU performance through memory hierarchy analysis (L1, L2, HBM data movement volumes); the roofline model [77] provides upper bounds, with recent LLM-specific extensions [32]. NeuSight [46] achieves 2.3% on GPT-3 by decomposing kernels into tiles that mirror CUDA's thread block tiling; Habitat [81] achieves 11.8% cross-GPU transfer via wave scaling.

The accuracy disparity across these approaches reflects a fundamental architectural distinction. Accelerator models achieve 5–10% error because DNN accelerator execution is deterministic: loop nest orderings fully determine data movement, and spatial architectures have predictable pipeline behavior. GPU execution introduces three sources of non-determinism that progressively degrade analytical accuracy: (1) warp scheduling decisions that depend on runtime resource availability, (2) memory coalescing patterns that depend on address alignment, and (3) L2 cache contention that depends on co-running kernels. AMALI's 23.6% MAPE reflects the cost of

Table 3: Summary of surveyed performance modeling tools for ML workloads, organized by target platform. Methodology: A=Analytical, S=Simulation, T=Trace-driven, M=ML-augmented, H=Hybrid. *Accuracy measures surrogate-vs-simulator fidelity, not real hardware error. †Reported accuracy unverifiable due to reproducibility issues. ‡No accuracy baseline against real hardware reported.

Tool	Platform	Method	Target	Accuracy	Speed	Key Capability
DNN Accelerator Modeling						
Timeloop [54]	NPU	A	Latency/Energy	5–10%	μs	Loop-nest DSE
MAESTRO [42]	NPU	A	Latency/Energy	5–15%	μs	Data-centric directives
Sparseloop [79]	NPU	A	Sparse tensors	5–10%	μs	Compression modeling
PyTorchSim [38]	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 [37]	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 [46]	GPU	H	Kernel/E2E latency	2.3%	ms	Tile-based prediction
Habitat [81]	GPU	H	Training time	11.8%	Per-kernel	Wave scaling
Distributed Training and LLM Serving						
ASTRA-sim [78]	Distributed	T	Training time	5–15%	Minutes	Collective modeling
SimAI [75]	Distributed	T	Training time	1.9%	Minutes	Full-stack simulation
Lumos [49]	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 [47]	Multi-GPU	T	DNN training	N/A‡	Minutes	Lightweight multi-GPU
Edge Device Modeling						
nn-Meter [83]	Edge	M	Latency	<1%†	ms	Kernel detection
LitePred [18]	Edge	M	Latency	0.7%	ms	85-platform transfer
HELP [45]	Multi	M	Latency	1.9%	ms	10-sample adaptation
Compiler Cost Models						
TVM [12]	GPU	M	Schedule perf.	~15%	ms	Autotuning guidance
Ansor [84]	GPU	M	Schedule perf.	~15%	ms	Program sampling
TLP [82]	GPU	M	Tensor program	<10%	ms	Transformer cost model

ignoring these dynamic effects; NeuSight's 2.3% captures them implicitly through tile-level profiling that matches the GPU's thread block scheduling granularity—predicting per-tile latency and aggregating, which naturally captures occupancy and memory locality that per-operator models miss.

LLM-specific and compiler models. VIDUR [3] simulates LLM serving at <5% error; LIFE [19], HERMES [5], Omniwise [23], and SwizzlePerf [74] target inference. TVM [12]/Ansor [84] (~15% MAPE), TLP [82] (<10%), and SynPerf [76] target compiler autotuning [85].

5.3 Distributed Training and LLM Serving

Distributed systems require modeling communication, synchronization, and parallelism strategies [29, 59, 68]. ASTRA-sim [78] achieves 5–15% error via Chakra traces [69]; SimAI [75] reaches 1.9% at Alibaba scale; Echo [8] scales simulation to 10K+ devices; Lumos [49] 3.3% on H100s; PRISM [21] provides prediction intervals at 10K+ GPUs. Paleo [58] pioneered analytical estimation; MAD Max [28] and Sailor [70] extend it; Llama 3 [15] provides validation ground truth at 16K GPUs. The speed hierarchy among distributed system simulators directly reflects their modeling granularity. VIDUR achieves second-scale simulation by modeling LLM serving at the request level—each prefill and decode phase is a single simulated event with profiled duration—sacrificing visibility into intra-phase behavior. ASTRA-sim operates at the collective communication level, replaying Chakra execution traces to model compute-communication overlap, which requires simulating each collective operation individually (minutes per configuration). SimAI further decomposes collectives to the NCCL algorithm level, modeling chunk-based ring and tree reduction protocols, which adds fidelity for network congestion effects at the cost of additional simulation time. The practical implication: practitioners exploring serving configurations (scheduler, batch size, model placement) should start with VIDUR's fast simulation, then validate promising configurations with ASTRA-sim or SimAI for network-sensitive scenarios.

For inference serving, VIDUR [3] models scheduling with vLLM [43]; DistServe [86] disaggregates prefill and decode for goodput optimization; Frontier [20] targets MoE; POD-Attention [24] and AQUA [67] address prefill-decode overlap and memory offloading respectively; ThrottLL'eM [35] models power effects; speculative decoding [9] creates a moving target for all simulators.

5.4 Edge Device Modeling

Hardware diversity makes per-device analytical modeling impractical. nn-Meter [83] claims <1% MAPE but is unverifiable due to dependency failures (Section 7); LitePred [18] achieves 0.7% across 85 platforms; HELP [45] reaches 1.9% with 10-sample meta-learning. ESM [52] 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.

5.5 Cross-Cutting Themes

Three architectural insights emerge from our analysis.

First, structural decomposition that mirrors hardware execution consistently outperforms black-box approaches. Timeloop's loop nests reflect systolic array dataflow, NeuSight's tiles mirror CUDA thread block scheduling, and VIDUR's prefill/decode split captures the GPU's distinct compute- vs. memory-bound regimes. In each case, the modeling abstraction succeeds because it aligns with the hardware boundary that dominates performance: data reuse at the PE array level, occupancy at the SM level, and phase-level batching at the system level. By contrast, AMALI's single-pass memory hierarchy model misses dynamic scheduling effects that cross these boundaries, explaining its higher error. Notably, tools with *verifiable* accuracy (e.g., Timeloop's reference outputs, VIDUR's Docker-based reproduction) appear more widely adopted than tools reporting high but unverifiable accuracy (e.g., nn-Meter).

Second, the most critical architectural features for accurate ML modeling differ by platform. For accelerators, data reuse (determined by dataflow and tiling) dominates because accelerator designs deliberately eliminate dynamic effects. For GPUs, thread block occupancy and memory coalescing are most critical because the SIMT execution model introduces contention not present in systolic arrays. For distributed systems, collective communication topology and pipeline bubble overhead dominate because compute per device is well-characterized but inter-device interaction is not. This explains why no single methodology works across all platforms.

Third, a persistent ***accuracy–generality–speed trade-off*** explains methodological diversity: cycle-accurate simulators (Accel-Sim, GPGPU-Sim) maximize accuracy by modeling microarchitectural state but sacrifice speed; analytical models (Timeloop, MAESTRO) maximize speed by exploiting structural regularity but sacrifice accuracy on dynamic workloads; ML-augmented approaches (nn-Meter, LitePred) achieve both speed and accuracy on trained distributions but sacrifice generality to unseen architectures. Subdomain maturity correlates with economic incentive: accelerator DSE is most mature (irreversible chip errors), distributed training is fastest-growing (million-dollar runs), and edge modeling has weakest reproducibility.

6 Comparison and Analysis

We analyze trade-offs across methodology types along accuracy and speed dimensions (see Table 3 for per-tool details); generalization and interpretability challenges are deferred to Section 8. Figure 5 visualizes the accuracy–speed trade-off space, revealing three distinct clusters of tools.

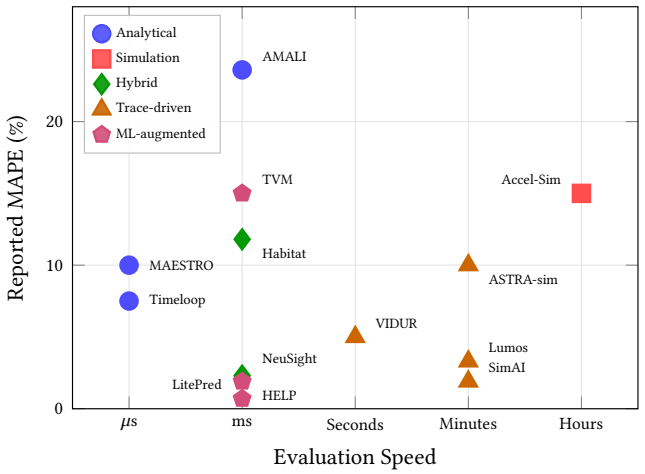

Figure 5: Accuracy–speed trade-off across surveyed tools. Each point represents a tool's reported MAPE vs. evaluation speed (log-scale categories). Hybrid (NeuSight) and trace-driven (SimAI) approaches achieve the best accuracy–speed balance.

6.1 Accuracy by Problem Difficulty

We organize accuracy results by inherent problem difficulty rather than comparing across incompatible benchmarks (Figure 6). Accelerator dataflow modeling is most tractable (Timeloop: 5–10%) because systolic arrays exhibit deterministic data movement—the absence of dynamic scheduling, speculative execution, and shared caches eliminates the primary sources of modeling error. Single-GPU kernel prediction achieves 2–12% via hybrid methods (NeuSight, Habitat), where the accuracy gap relative to accelerators arises from GPU-specific dynamic effects: warp scheduling decisions that depend on runtime register pressure, memory coalescing efficiency that varies with access patterns, and shared memory bank conflicts that are input-dependent. Distributed systems reach 2–15% (SimAI 1.9%, ASTRA-sim 5–15%), where the dominant error source shifts from compute modeling to communication topology and collective algorithm selection. Cross-platform edge prediction achieves 0.7–2% but requires per-device profiling; GPU analytical modeling remains hardest (AMALI: 23.6%). Setup costs vary dramatically: analytical models require only architecture specifications, ML-augmented approaches need 10–10K profiling samples per device, and cycle-accurate simulators require hardware-specific binaries or traces.

6.2 Practitioner Tool Selection

Tool selection depends on the target platform, acceptable error margin, and available setup time; Figure 7 provides a decision flowchart. For *accelerator DSE*, use Timeloop or MAESTRO for microsecond-speed exhaustive search with interpretable bottleneck feedback; Sparseloop extends this to sparse workloads. For *GPU evaluation*, NeuSight offers the best accuracy–speed balance for LLMs; use Accel-Sim when microarchitectural detail is needed, accepting the

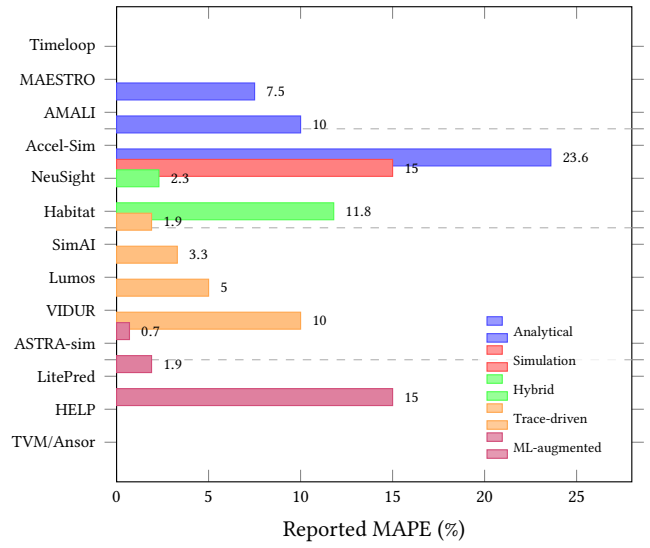

Figure 6: Reported accuracy (MAPE) of surveyed tools, grouped by methodology type. Range midpoints used where ranges are reported. Cross-tool comparison is approximate due to differing benchmarks, workloads, and hardware targets.

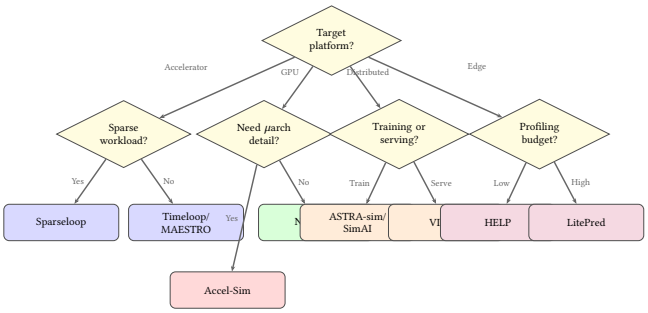

Figure 7: Tool selection decision flowchart. Practitioners choose based on target platform, then refine by workload characteristics and resource constraints. Colors indicate methodology type: blue=analytical, green=hybrid, orange=trace-driven, purple=ML-augmented.

1000× slowdown. For *distributed systems*, use VIDUR for LLM serving configuration and ASTRA-sim or SimAI for training parallelism at scale; MAD Max provides fast analytical estimates when trace collection is impractical. For *edge devices*, LitePred offers the broadest platform coverage, while HELP excels with minimal profiling data. Practitioners should consider tools with Docker-first deployment (VIDUR, Timeloop, ASTRA-sim) over tools with unpinned dependencies, as our evaluation shows containerized tools are consistently easier to reproduce.

Table 4: Reproducibility evaluation results. Tools are ranked by overall assessment. †Timeloop CLI works but Python bindings fail.

Tool	Setup	Reprod.	Usability	Total
VIDUR	2.5	3.5	3	9/10
Timeloop†	3	4	2	9/10
ASTRA-sim	2.5	3	3	8.5/10
NeuSight	2	3	2.5	7.5/10
nn-Meter	2	0	1	3/10

Table 5: VIDUR simulation results for Llama-2-7B inference serving on a simulated A100 GPU (100 requests each, seed=42). Schedulers use different arrival rates, so latency values are not directly comparable; results illustrate VIDUR's scheduling model fidelity. All metrics from our own experiments.

Metric	vLLM	Sarathi
Requests	100	100
QPS (Poisson)	2.0	4.0
Avg E2E latency (s)	0.170	0.174
P99 E2E latency (s)	0.285	0.294
Avg TTFT (s)	0.027	0.028
Avg TPOT (s)	0.0093	0.0095
Requests preempted	28	0

7 Experimental Evaluation

We conducted hands-on evaluations of five tools spanning methodology types: Timeloop (analytical), ASTRA-sim (trace-driven, distributed), VIDUR (trace-driven, LLM serving), nn-Meter (ML-augmented, edge), and NeuSight (hybrid, GPU).

Environment. All evaluations ran on Apple M2 Ultra (aarch64, 192 GB RAM) using Docker containers where provided—no GPU hardware was available, so we cannot validate absolute accuracy claims. We assess each tool on setup difficulty, output reproducibility, and usability. Table 4 summarizes results.

7.1 Per-Tool Results

VIDUR (9/10). We simulated Llama-2-7B on a simulated A100 under two scheduler configurations (Table 5). Note that the two schedulers were run at different arrival rates (QPS 2.0 vs. 4.0), so their latency metrics are *not directly comparable*; rather, the results illustrate VIDUR's ability to model distinct scheduling behaviors. The vLLM scheduler preempted 28% of requests even at lower load, while Sarathi's chunked prefill [2] avoided preemptions entirely despite 2× higher arrival rate—consistent with the KV-cache management differences described in the respective papers [2, 43].

Timeloop (9/10). Docker CLI produces deterministic, bit-identical outputs for Eyeriss-like configurations; reference outputs enable hardware-free verification. Python bindings fail (`ImportError: libbarvinok.so.23`).

ASTRA-sim (8.5/10). We ran collective microbenchmarks and ResNet-50 training at 2–8 GPUs (Table 6). Reduce-Scatter takes

Table 6: ASTRA-sim quantitative results from our experiments on the HGX-H100 configuration. Top: collective microbenchmarks (8 NPUs, 1 MB). Bottom: ResNet-50 data-parallel training 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%

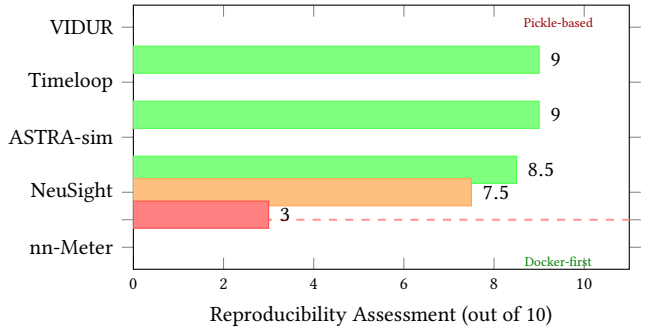

Figure 8: Reproducibility assessment for evaluated tools. Docker-first tools (VIDUR, Timeloop, ASTRA-sim) are consistently reproducible, while tools relying on serialized ML models (nn-Meter) become unusable. The dashed line separates Docker-based from non-Docker deployments.

half the time of All-Reduce (consistent with half the data); communication overhead scales 5.76× for 4× more GPUs, matching ring All-Reduce scaling.

NeuSight (7.5/10). Tile-based decomposition mirrors CUDA tiling for dense operations; irregular workloads had limited examples.

nn-Meter (3/10). After four attempts (>4h), no predictions ran: pickle-serialized predictors (scikit-learn 0.23.1) are incompatible with current versions. The claimed <1% MAPE is **unverifiable**.

Figure 8 visualizes the reproducibility assessment, showing that Docker-first tools are consistently easier to reproduce.

7.2 Lessons and Threats to Validity

Five lessons emerge: (1) **Docker-first deployment** correlates with high reproducibility in our sample (all three Docker-based tools produced verifiable outputs; nn-Meter without Docker did not), though our sample of five tools limits causal conclusions. (2) **ML model serialization is fragile**—nn-Meter's pickle-based predictors became unusable within two years. (3) **Reference outputs enable**

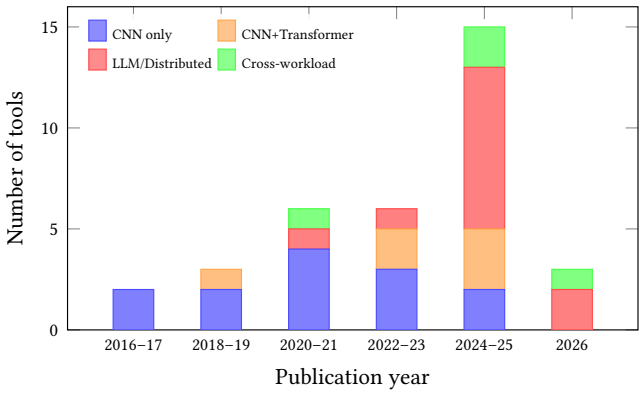

Figure 9: Workload coverage of surveyed tools by publication period. The shift toward transformer and LLM workloads accelerates from 2023, but MoE and diffusion models remain largely uncharacterized.

trust without hardware—Timeloop and ASTRA-sim include verifiable baselines. (4) **Scale-limited evaluation understates system tools**—our 2–8 GPU tests show only 0.30% communication overhead, far below production scales [15]. (5) **Reproducible accuracy claims should be weighted higher** than unreproducible ones.

Threats. Our venue-focused search may under-represent industry and non-English publications; we exclude proprietary tools (Nsight Compute, internal TPU models); and accuracy metrics vary across papers (MAPE, RMSE, Kendall's τ), limiting direct comparison.

8 Open Challenges and Future Directions

Generalization gaps. *Workload*: CNN→transformer transfer is largely unvalidated (NeuSight excepted); MoE, diffusion [39], and dynamic inference lack validated tools; scaling laws [14, 22, 27, 36] predict loss but not latency. Figure 9 shows the shift toward LLM workloads since 2023. *Hardware*: cross-family transfer (GPU→TPU→PIM) remains unsolved despite meta-learning (HELP) and feature-based transfer (LitePred). *Temporal*: software stack evolution silently invalidating models is addressed by no tool.

The composition problem. Composing kernel-level predictions into end-to-end estimates is unsolved (Figure 10): NeuSight's 2.3% kernel MAPE yields ~10× higher variance at model level ($\sigma_{\text{model}} \approx \sigma_{\text{kernel}} \cdot \sqrt{N}$), and correlated errors can compound linearly. VIDUR sidesteps this by profiling entire prefill/decode phases.

Emerging hardware and reproducibility. PIM [26, 31, 44, 55], chiplets, and disaggregated designs blur memory hierarchy assumptions; FlashAttention [16] changes the landscape faster than models retrain. No MLPerf [51, 63] equivalent exists for performance *prediction*.

Future directions: (1) validated non-CNN tools; (2) bounded composition error; (3) unified energy-latency-memory prediction [62]; (4) temporal robustness benchmarks; (5) Docker-first deployment with portable formats (ONNX, Chakra [69]).

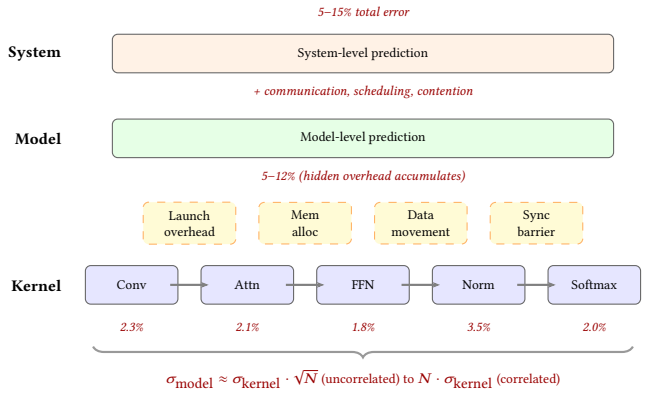

Figure 10: Error composition across abstraction levels. Kernel-level predictions (2–3% each) accumulate through hidden overheads (kernel launch, memory allocation, data movement, synchronization) that are not captured by kernel-level tools, yielding 5–12% model-level error. System-level errors add communication and scheduling overhead.

9 Conclusion

This survey analyzed 22 tools in depth for predicting ML workload performance, organized by methodology type, target platform, and abstraction level. Key findings: (1) *No single methodology dominates*—analytical models offer microsecond interpretable evaluation, trace-driven simulators provide 2–15% system-level error, and hybrid approaches achieve the best accuracy–speed balance (NeuSight: 2.3% MAPE), with the right choice depending on the practitioner's priorities. (2) *LLM workloads demand specialized modeling*—prefill/decode distinctions, KV cache management, and dynamic batching require purpose-built tools (VIDUR, Frontier) rather than CNN-era extensions. (3) *Reproducibility is a practical bottleneck*—Docker-first tools remain reproducible while tools relying on serialized ML models have become unusable. (4) *Accuracy claims require scrutiny* due to varying benchmarks and metrics.

The most pressing gaps are CNN-to-transformer generalization, kernel-to-end-to-end composition, emerging hardware support (PIM, chiplets), and reproducibility failures. As ML workloads grow in scale and diversity, this survey provides practitioners guidance for tool selection and researchers a roadmap for advancing the field.

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