

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

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Abstract

As machine learning workloads grow in scale and complexity—spanning training and inference for CNNs, transformers, mixture-of-experts models, and LLMs—architects and system designers need fast, accurate methods to predict their performance across diverse hardware platforms. This survey provides a comprehensive analysis of the tools and methods available for modeling and simulating the performance of ML workloads, covering analytical models, cycle-accurate simulators, trace-driven approaches, and ML-augmented hybrid techniques. We survey over 30 tools drawn from 53 papers across architecture venues (MICRO, ISCA, HPCA, ASPLOS) and systems venues (MLSys, OSDI, NSDI) published between 2016–2026, spanning DNN accelerator modeling (Timeloop, MAESTRO, Sparseloop), GPU simulation (GPGPU-Sim, Accel-Sim, NeuSight), distributed training simulation (ASTRA-sim, Lumos, SimAI), and LLM inference serving (VIDUR, Frontier, AMALI). We organize the literature along three dimensions—methodology type (analytical, simulation, ML-augmented, hybrid), target platform (accelerators, GPUs, distributed systems, edge devices), and abstraction level (kernel, model, system)—while additionally characterizing tools by workload coverage, revealing a pervasive CNN-validation bias. Our analysis reveals that hybrid approaches combining analytical structure with learned components achieve the best accuracy-speed trade-offs, while pure analytical models offer superior interpretability for design space exploration. We conduct hands-on reproducibility evaluations of five representative tools, finding that reproducibility varies dramatically: Docker-first tools score 8.5+/10 on our rubric while tools relying on serialized ML models risk becoming unusable. We identify key open challenges including cross-workload generalization beyond CNNs, composition of kernel-level predictions to end-to-end accuracy, and support for emerging architectures. This survey provides practitioners guidance for selecting appropriate modeling tools and researchers a roadmap for advancing the field of ML workload performance prediction.

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—spanning training and inference for CNNs, transformers, mixture-of-experts models, and graph neural networks—have become the dominant consumers of compute

across datacenters and edge devices. The shift toward domain-specific architectures [22], from Google’s TPU [30, 31] to custom training accelerators, has created a heterogeneous hardware landscape where architects and system designers need fast, accurate performance predictions to navigate vast design spaces, select parallelization strategies, provision serving infrastructure, and optimize hardware-software co-design. Yet ML workloads pose unique modeling challenges: they exhibit diverse computational patterns (dense matrix operations in attention layers, sparse accesses in GNNs, communication-bound collective operations in distributed training) across this increasingly heterogeneous landscape of GPUs, TPUs, custom accelerators, and multi-device clusters.

A rich ecosystem of modeling and simulation tools has emerged to address these challenges, spanning a methodological spectrum from analytical models to cycle-accurate simulators to ML-augmented hybrid approaches. Analytical frameworks like Timeloop [50] and MAESTRO [38] model DNN accelerator performance through closed-form data movement analysis, achieving 5–10% error versus RTL at microsecond evaluation speed. Cycle-accurate simulators like GPGPU-Sim [4] and Accel-Sim [34] provide detailed GPU modeling but require hours per workload. Trace-driven simulators like ASTRA-sim [71] and VIDUR [3] target distributed training and LLM serving at system scale. ML-augmented approaches like NeuSight [42] learn performance functions from profiling data, achieving 2.3% error on GPU kernel prediction. Each methodology occupies a distinct point in the accuracy-speed-generality trade-off space.

Despite this rich tool landscape, no comprehensive survey organizes these methods from the perspective of the ML workload practitioner—the architect or engineer who needs to select a modeling tool for a specific design or deployment task. Existing surveys focus on ML *techniques* for performance modeling [65] or on specific hardware targets [50], leaving practitioners without guidance on which tools suit their needs across the full modeling spectrum. This survey fills that gap by providing a methodology-centric view of the tools and methods available for predicting ML workload performance.

We make the following contributions:

- A **methodology-centric taxonomy** organizing tools along three dimensions: methodology type (analytical, simulation, ML-augmented, hybrid), target platform (DNN accelerators, GPUs, distributed systems, edge devices), and abstraction level (kernel, model, system), with a quantitative coverage matrix identifying research gaps and a workload coverage analysis exposing the CNN-validation bias in the literature.
- A **systematic survey** of over 30 modeling tools drawn from 53 papers across architecture venues (MICRO, ISCA,

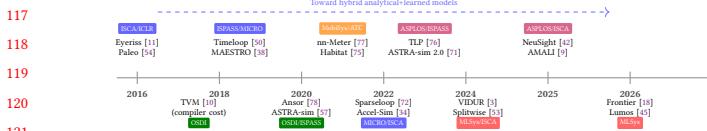


Figure 1: Evolution of performance modeling tools for ML workloads (2016–2026). Early analytical frameworks (EyeRISS, Paleo) gave way to systematic accelerator modeling (Timeloop, MAESTRO) and distributed training simulation (ASTRA-sim). ML-augmented approaches (TVM, Habitat, NeuSight) learn performance functions from data. Recent work targets LLM-specific modeling (VIDUR, AMALI, Frontier) and large-scale training prediction (Lumos).

HPCA, ASPLoS) and systems venues (MLSys, OSDI, NSDI) published between 2016–2026, using documented selection criteria.

- A **comparative analysis** examining trade-offs between accuracy, speed, generalization, and interpretability, with careful qualification of paper-reported accuracy claims and identification of cases where reported numbers are unverifiable.
- **Hands-on reproducibility evaluations** of representative tools with a 10-point rubric, and identification of **open challenges** including the CNN-to-transformer generalization gap, kernel-to-end-to-end error composition, and emerging accelerator support.

The remainder of this paper is organized as follows. Section 2 describes our survey methodology and positions this work relative to existing surveys. Section 3 provides background on ML workload characteristics and modeling fundamentals. Section 4 presents our classification taxonomy. Section 5 surveys approaches organized by target platform. Section 6 offers comparative analysis across key dimensions and a practitioner tool selection guide. Section 7 presents hands-on reproducibility evaluations. Section 8 discusses open challenges and future directions. Section 9 concludes.

Figure 1 illustrates the evolution of performance modeling tools for ML workloads, from early analytical frameworks through simulators 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, IPASS). 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).

2.1 Related Surveys

Prior surveys address adjacent topics: Rakhshanfar and Zarandi [56] survey ML for processor DSE; Sze et al. [66] treat DNN hardware design (the foundation for Timeloop/MAESTRO); GPGPU-Sim [4] and gem5 [6] have extensive evaluation literature; and MLPPerf [47, 59] standardizes *measurement* rather than *prediction*. This survey differs by spanning the full methodology spectrum across all major platforms with hands-on reproducibility evaluations. The closest prior work, Dudziak et al. [15], compares edge device predictors for NAS; we broaden to the full landscape.

3 Background

3.1 ML Workload Characteristics

ML workloads, defined as computation graphs in frameworks like PyTorch [52] and TensorFlow [1], present distinct modeling challenges. Their operators (convolutions, matrix multiplications, attention) have statically known shapes amenable to analytical modeling, though mixture-of-experts and dynamic inference introduce input-dependent control flow. Performance is highly sensitive to how tensors map onto specialized memory hierarchies (dataflow, tiling, loop ordering), and for LLM inference, KV cache management dominates memory behavior [39]. At scale, training distributes across thousands of GPUs via data, tensor, pipeline, and expert parallelism [13], requiring system-level modeling of compute–memory–network interactions. LLM inference further splits into compute-bound prefill and memory-bound decode phases [53], both of which must be modeled under batched serving [2, 74].

3.2 Modeling Methodologies

We classify approaches into four categories forming our taxonomy’s primary axis. **Analytical models** express performance as closed-form functions—e.g., the roofline model [70] bounds throughput by $P = \min(\pi, \beta \cdot I)$, while Timeloop [50] computes data movement costs for DNN accelerator mappings. They offer microsecond evaluation but require per-architecture derivation. **Cycle-accurate simulators** (gem5 [6], GPGPU-Sim [4], Accel-Sim [34]) achieve high fidelity but at 1000–10000× slowdown; sampling techniques [61, 73] help but were not designed for ML workloads. **Trace-driven simulators** like ASTRA-sim [71] (distributed training via Chakra traces [63]) and VIDUR [3] (LLM serving) trade some fidelity for orders-of-magnitude speedup. **ML-augmented approaches** learn performance functions from profiling data, ranging from random forests (nn-Meter [77]) and XGBoost (TVM [10]) to deep learning (NeuSight [42]) and meta-learning (HELP [41]); they capture non-linear relationships but may not generalize beyond their training distribution.

3.3 Problem Formulation

Performance modeling maps workload \mathcal{W} and hardware \mathcal{H} to a metric y : $\hat{y} = f(\mathcal{W}, \mathcal{H}; \theta)$, with workloads represented at operator, graph, IR, or trace level, and hardware characterized by specifications, counters, or learned embeddings. Prediction targets include latency, throughput, energy, and memory footprint. Accuracy metrics—MAPE, RMSE, and rank correlation (Kendall’s τ)—vary

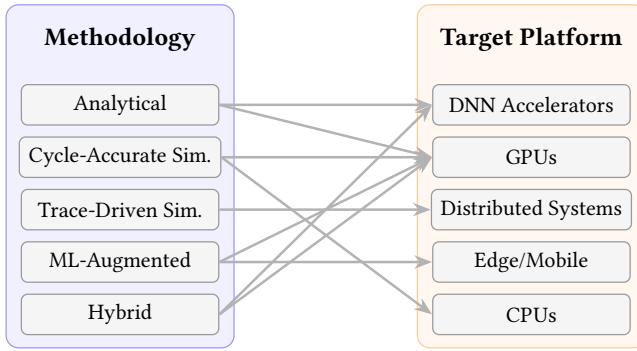


Figure 2: Primary dimensions of the taxonomy for ML workload performance modeling. The primary axis is methodology type (how performance is predicted); the secondary axis is target platform. The third dimension, abstraction level, is shown separately in Figure 3. Arrows show dominant pairings: analytical models for accelerators, cycle-accurate simulation for GPUs/CPUs, trace-driven simulation for distributed systems, and ML-augmented approaches for edge devices and compiler cost models.

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.

Figure 2 illustrates the primary and secondary dimensions. Table 1 provides a unified view combining the coverage matrix (number of surveyed tools per methodology–platform cell) with trade-off profiles (evaluation speed, data requirements, interpretability, and failure modes), with empty cells highlighting research gaps.

Table 1 reveals three structural observations. First, trace-driven simulation is exclusively used for distributed systems—no surveyed tool applies trace-driven methods to single-device GPU or accelerator modeling, despite the potential for trace-driven approaches to avoid the slowdown of cycle-accurate simulation while retaining more fidelity than analytical models. Second, edge/mobile devices are served exclusively by ML-augmented approaches; the absence of analytical or hybrid models for edge devices reflects the hardware diversity problem but also represents a research gap, since hybrid approaches could combine the interpretability of analytical models with the adaptability of learned components. Third, no ML-augmented or hybrid tool specifically targets distributed system modeling—tools like VIDUR use ML internally for kernel prediction but are architecturally trace-driven simulators. The trade-off columns further show that methodologies cluster into two speed

regimes: sub-millisecond (analytical, ML-augmented, hybrid) suitable for design space exploration, and minutes-to-hours (simulation, trace-driven) suitable for detailed validation.

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.

Analytical models express performance as closed-form functions of workload and hardware parameters. Timeloop [50] achieves 5–10% error versus RTL at 2000 \times speedup for DNN accelerators; MAESTRO [38] and Sparseloop [72] extend to data-centric directives and sparse tensors; Paleo [54] and AMALI [9] target distributed training and GPU LLM inference, respectively. These models provide microsecond evaluation and full interpretability but require per-architecture derivation and may miss dynamic effects (AMALI’s 23.6% MAPE illustrates this ceiling for GPUs).

Cycle-accurate simulators model hardware at register-transfer level. GPGPU-Sim [4] and Accel-Sim [34] achieve 0.90–0.97 IPC correlation; PyTorchSim [35] integrates PyTorch 2 with NPU simulation. Speed (1000–10000 \times slowdown) makes these impractical for ML design space exploration; sampling techniques [60, 61, 73] help but are unvalidated for ML workloads.

Trace-driven simulators replay execution traces for system-level modeling. ASTRA-sim [71] achieves 5–15% error for distributed training via Chakra traces [63]; VIDUR [3] provides <5% error for LLM serving; SimAI [68], Lumos [45], and Frontier [18] target large-scale training and MoE inference. Some tools use ML internally (e.g., VIDUR’s random forests for kernel prediction), blurring the boundary with hybrid approaches.

ML-augmented models learn performance functions from profiling data: nn-Meter [77] (random forests for edge devices), LitePred [16] (85-platform transfer), HELP [41] (10-sample meta-learning), and TVM [10]/Ansol [78] (compiler autotuning with TenSet [79]). Their critical failure mode is *silent distribution shift*—CNN-trained models may produce confident but wrong predictions for transformers.

Hybrid analytical+ML models combine physics-based priors with learned residual corrections. NeuSight [42] achieves 2.3% MAPE on GPT-3 inference via tile-based prediction; Concorde [49] achieves 2% CPI error on CPUs; Habitat [75] decomposes compute/memory components; ArchGym [37] connects ML surrogates to analytical simulators. Transfer learning provides 22.5% average improvement [15].

4.2 Secondary Axes: Platform and Abstraction Level

The target platform constrains applicable methodologies: **DNN accelerators** [30, 31] are best served by analytical models (Timeloop, MAESTRO, Sparseloop) due to regular memory hierarchies; **GPUs** span the full methodology spectrum reflecting SIMD complexity; **distributed systems** require trace-driven simulation (ASTRA-sim, VIDUR, SimAI) for collective communication and pipeline parallelism; **edge/mobile devices** are dominated by ML-augmented approaches (nn-Meter, LitePred, HELP) due to hardware diversity;

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	μ s	None	High	Dynamic effects
Cycle-Accurate	1	2	0	0	1	Hours	Binary	High	Scale
Trace-Driven	0	0	7	0	0	Min.	Traces	Med.	Trace fidelity
ML-Augmented	0	3	0	3	1	ms	Profiling	Low	Distrib. shift
Hybrid	1	2	0	0	1	ms	Mixed	Med.	Training domain

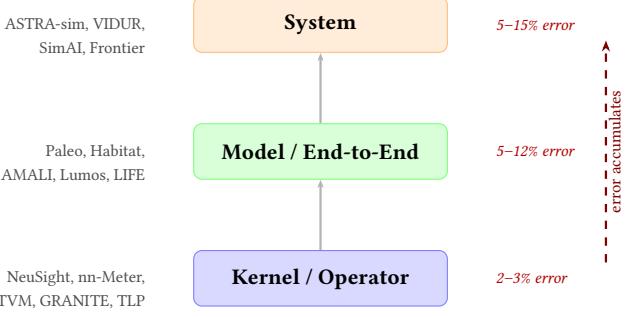


Figure 3: Abstraction level hierarchy and the composition problem. Tools operate at one of three levels; composing predictions across levels accumulates error. Error ranges are representative values from surveyed papers.

and CPUs are less studied for ML workloads (Concorde [49], GRANITE [65]).

Abstraction level determines where composition errors arise. **Kernel-level** tools (NeuSight, nn-Meter, TVM) achieve 2–3% error but composing predictions into end-to-end latency introduces errors from memory allocation, kernel launch overhead, and inter-operator data movement. **Model-level** tools (Paleo, Habitat, AMALI) account for graph-level effects at 5–12% error. **System-level** tools (ASTRA-sim, VIDUR, SimAI) capture communication and scheduling at 5–15% error, with kernel-level errors propagating through the composition chain. Figure 3 illustrates this hierarchy.

4.3 Workload Coverage

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

The table reveals that **no surveyed tool has been validated on diffusion models or dynamic inference workloads** [36], only Frontier [18] has validated MoE support, and no single tool offers 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.

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

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

DNN accelerators employ specialized dataflows and memory hierarchies optimized for tensor operations [66], and their computational regularity makes this domain particularly amenable to analytical modeling.

Analytical frameworks dominate. Timeloop [50] computes data reuse, latency, and energy from loop-nest representations at 5–10% error versus RTL simulation with 2000× speedup, and provides deterministic reference outputs for standard designs (Eyeriss [11], Simba). MAESTRO [38] simplifies specification via data-centric directives but is less precise for energy modeling. Sparseloop [72] extends Timeloop to sparse tensors by modeling sparsity patterns, compression formats (CSR, bitmap), and hardware intersection

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
<i>DNN Accelerator Modeling</i>						
Timeloop [50]	NPU	A	Latency/Energy	5–10%	μs	Loop-nest DSE
MAESTRO [38]	NPU	A	Latency/Energy	5–15%	μs	Data-centric directives
Sparseloop [72]	NPU	A	Sparse tensors	5–10%	μs	Compression modeling
PyTorchSim [35]	NPU	S	Cycle-accurate	N/A [‡]	Hours	PyTorch 2 integration
ArchGym [37]	Multi	H	Multi-objective	0.61%*	ms	ML-aided DSE
<i>GPU Performance Modeling</i>						
Accel-Sim [34]	GPU	S	Cycle-accurate	10–20%	Hours	SASS trace-driven
GPGPU-Sim [4]	GPU	S	Cycle-accurate	10–20%	Hours	CUDA workloads
AMALI [9]	GPU	A	LLM inference	23.6%	ms	Memory hierarchy
NeuSight [42]	GPU	H	Kernel/E2E latency	2.3%	ms	Tile-based prediction
Habitat [75]	GPU	H	Training time	11.8%	Per-kernel	Wave scaling
<i>Distributed Training and LLM Serving</i>						
ASTRA-sim [71]	Distributed	T	Training time	5–15%	Minutes	Collective modeling
SimAI [68]	Distributed	T	Training time	1.9%	Minutes	Full-stack simulation
Lumos [45]	Distributed	T	LLM training	3.3%	Minutes	H100 training
VIDUR [3]	GPU cluster	T	LLM serving	<5%	Seconds	Prefill/decode phases
Frontier [18]	Distributed	T	MoE inference	—	Minutes	Stage-centric sim.
TrioSim [43]	Multi-GPU	T	DNN training	N/A [‡]	Minutes	Lightweight multi-GPU
<i>Edge Device Modeling</i>						
nn-Meter [77]	Edge	M	Latency	<1% [†]	ms	Kernel detection
LitePred [16]	Edge	M	Latency	0.7%	ms	85-platform transfer
HELP [41]	Multi	M	Latency	1.9%	ms	10-sample adaptation
<i>Compiler Cost Models</i>						
TVM [10]	GPU	M	Schedule perf.	~15%	ms	Autotuning guidance
Ansor [78]	GPU	M	Schedule perf.	~15%	ms	Program sampling
TLP [76]	GPU	M	Tensor program	<10%	ms	Transformer cost model

units—critical for transformer inference but limited to static, known sparsity distributions.

Simulation and ML-augmented approaches. PyTorchSim [35] integrates PyTorch 2 with cycle-accurate NPU simulation, directly consuming computation graphs to eliminate manual workload translation, but does not report real-hardware accuracy and inherits simulation speed limitations. ArchGym [37] connects ML surrogates to analytical simulators for design space exploration; its 0.61% RMSE measures surrogate-vs-simulator fidelity, not real-hardware accuracy. Early PIM modeling tools [23, 28, 40, 51] target attention acceleration and PIM-GPU co-simulation but lack real PIM hardware validation (Section 8).

Synthesis. Accelerator modeling is the most mature subdomain, with Timeloop achieving a favorable accuracy–speed–interpretability balance as the de facto DSE standard. The progression from Timeloop through Sparseloop to PIM-aware tools illustrates a recurring pattern: each extension addresses a new workload characteristic but erodes the simplicity advantage of analytical approaches. The key gap is silicon validation—neither ArchGym nor PyTorchSim validates against manufactured hardware, leaving all accelerator tools anchored to RTL comparisons.

5.2 GPU Performance Modeling

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

Cycle-accurate simulation. GPGPU-Sim [4] and Accel-Sim [34] achieve 0.90–0.97 IPC correlation; recent reverse-engineering of modern GPU cores [27] improved Accel-Sim to 13.98% MAPE. However, 1000–10000× slowdown makes these tools impractical at production scale.

Analytical models. The roofline model [70] provides upper bounds but misses dynamic effects; Roofline-LLM [29] extends it to LLM inference. AMALI [9] reduces LLM inference MAPE from 127% to 23.6% via memory hierarchy modeling—the residual error reflects the fundamental difficulty of analytically capturing GPU dynamic behavior (warp scheduling, cache contention).

Hybrid learned models. NeuSight [42] achieves 2.3% MAPE on GPT-3 inference (H100/A100/V100) via tile-based prediction mirroring CUDA execution. Habitat [75] uses wave scaling to decompose compute and memory components, achieving 11.8% cross-GPU transfer error (e.g., V100→A100), but requires source GPU profiling and assumes occupancy patterns remain similar across generations. Direct comparison requires caution: NeuSight targets 2023–2025

hardware with LLMs, while Habitat was designed for earlier GPUs with CNNs.

LLM-specific modeling. LLM execution exhibits distinct pre-fill (compute-bound) and decode (memory-bound) phases [53, 80]. VIDUR [3] simulates LLM serving with scheduling strategies (Orca [74], Sarathi [2]) at <5% error. LIFE [17] provides hardware-agnostic analytical inference modeling; HERMES [5] targets heterogeneous disaggregated serving; and emerging predictors include Omniwise [21] and SwizzlePerf [67].

Compiler cost models. TVM [10] and Ansor [78] use ML cost models for autotuning at ~15% MAPE, with TenSet [79] enabling pre-training. TLP [76] uses transformer-based modeling for irregular workloads at <10% MAPE. SynPerf [69] uses performance models to guide kernel synthesis; both SwizzlePerf and SynPerf prioritize ranking accuracy over absolute error.

Synthesis. GPU modeling exhibits the widest methodological spread: cycle-accurate simulation, analytical models, hybrid learned approaches, and LLM-based predictors all target the same hardware with error rates spanning 2%–24%. This diversity reflects the fundamental tension between microarchitectural complexity (making analytical modeling hard) and rapid hardware evolution (invalidating training data for learned approaches). NeuSight currently offers the best accuracy–speed trade-off for LLM workloads, but per-GPU profiling limits pre-silicon use—a gap that AMALI and LIFE fill despite higher error. The compiler cost model ecosystem (TVM, TLP, SynPerf) represents a distinct use case where relative ranking matters more than absolute prediction.

5.3 Distributed Training and LLM Serving

Distributed systems introduce communication overhead, synchronization barriers, and parallelism strategy choices across tensor [62], pipeline [26], and data parallelism with memory-efficient optimizers [55].

Training simulation. ASTRA-sim [71] provides end-to-end training simulation via Chakra traces [63] at 5–15% error versus HGX-H100 clusters. SimAI [68] achieves 1.9% MAPE at Alibaba Cloud scale; Lumos [45] achieves 3.3% error on H100 training; Echo [7] and TrioSim [43] offer additional training simulation approaches. PRISM [19] produces prediction intervals at 10K+ GPU scale, capturing stochastic variation.

Scaling and parallelism. Paleo [54] pioneered analytical training-time estimation; MAD Max [25] extends this per parallelism dimension. The Llama 3 scaling study [13] documents 4D parallelism at 16K H100 GPUs as validation ground truth. Sailor [64] addresses parallelism selection over heterogeneous clusters.

Inference serving. VIDUR [3] extends to distributed serving with vLLM [39] scheduling; Frontier [18] targets MoE and disaggregated inference; ThrottLL'eM [32] models GPU power management effects on inference. KV cache management is the key serving bottleneck (vLLM's PagedAttention [39] achieves 2–4× throughput), modeled by VIDUR at the system level; low-level memory simulators (DRAMSim3 [44], Ramulator 2 [46]) integrate with tools like Accel-Sim for detailed memory modeling. Algorithmic innovations like speculative decoding [8] create a moving-target challenge for all serving simulators.

Synthesis. Distributed modeling is the fastest-growing subdomain, bifurcating into *trace-driven fidelity* (ASTRA-sim, SimAI) and *analytical decomposition* (Paleo, MAD Max), with PRISM's probabilistic approach as an emerging third path.

5.4 Edge Device Modeling

Edge devices impose strict power, memory, and latency constraints, and their hardware diversity (mobile CPUs, GPUs, NPUs, DSPs) makes per-device analytical modeling impractical, driving ML-augmented approaches.

nn-Meter [77] reports <1% MAPE using random forest ensembles, but this claim is unverifiable: pre-trained predictors fail with modern scikit-learn versions, scoring 3/10 in our reproducibility evaluation. LitePred [16] achieves 0.7% MAPE across 85 platforms using VAE-based intelligent sampling that reduces adaptation to under one hour per device, though the platforms are predominantly ARM-based and transfer to NPUs/DSPs likely degrades. HELP [41] achieves 1.9% MAPE with MAML-style 10-sample adaptation, though accuracy depends on selecting representative operators for the target workload. ESM [48] systematically evaluates surrogate models for hardware-aware NAS, finding that well-tuned random forests match deep learning surrogates—suggesting the field may over-invest in model complexity relative to data quality. The latency predictor study [15] shows transfer learning provides 22.5% average improvement, up to 87.6% on challenging cross-platform transfers.

Synthesis. Edge modeling is dominated by ML-augmented approaches, with the central challenge being *generalization* to new devices with minimal profiling. ESM's finding that simple models match complex ones, combined with nn-Meter's reproducibility failure, suggests that data quality and tool longevity matter more than model sophistication.

5.5 Cross-Cutting Themes

Several themes cut across platform categories. *Structural decomposition* mirroring hardware execution outperforms black-box approaches (Timeloop's loop nests, NeuSight's tiles, VIDUR's pre-fill/decode separation), while modular pluggable backends (ASTRA-sim, VIDUR) enable adoption. *Verifiable moderate accuracy* matters more than *unverifiable high accuracy*—Timeloop (9/10 reproducibility) and ASTRA-sim (8.5/10) see sustained adoption, while nn-Meter (<1% MAPE claimed, 3/10 reproducibility) sees decline.

A persistent **accuracy–generality–speed trilemma** explains why no single methodology has displaced others: cycle-accurate simulators maximize accuracy but sacrifice speed; analytical models maximize speed but sacrifice accuracy on complex hardware; ML-augmented approaches achieve both but sacrifice generality, requiring retraining when hardware changes. The maturity of each subdomain mirrors economic incentive: accelerator DSE is most mature (irreversible chip design errors), distributed training simulation is fastest-growing (million-dollar training runs), and edge modeling has weakest reproducibility (lower deployment costs).

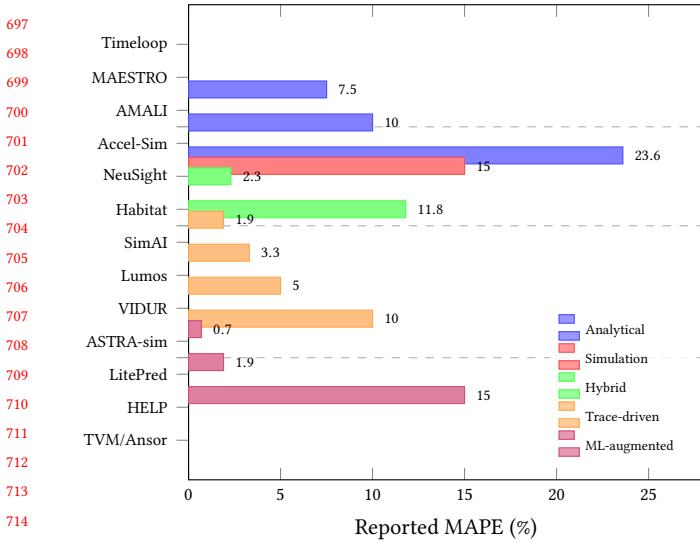


Figure 4: Reported accuracy (MAPE) of surveyed tools, grouped by methodology type. Range midpoints used where ranges are reported. Cross-tool comparison is approximate due to differing benchmarks, workloads, and hardware targets.

6 Comparison and Analysis

We analyze trade-offs across methodology types along accuracy, speed, generalization, and interpretability. Table 4 summarizes characteristics of representative tools.

6.1 Accuracy by Problem Difficulty

Rather than comparing accuracy directly across different benchmarks and metrics, we organize results by problem difficulty. **Accelerator dataflow modeling** is most amenable to prediction (Timeloop: 5–10% error via purely analytical means). **Single-GPU kernel prediction** achieves 2–12% error through hybrid approaches (NeuSight, Habitat). **Distributed system-level prediction** achieves 2–15% error (SimAI 1.9%, Lumos 3.3%, ASTRA-sim 5–15%). **Cross-platform edge prediction** achieves 0.7–2% error (LitePred, HELP) but requires per-device profiling. **GPU analytical modeling** remains hardest (AMALI: 23.6% MAPE for LLM inference).

Figure 4 visualizes reported MAPE across tools. Hybrid approaches achieve the lowest error on GPU workloads, trace-driven simulators cluster at 2–15% for distributed systems, and analytical models trade accuracy for speed.

6.2 Generalization and Interpretability

Workload generalization remains the primary challenge: nearly all accuracy numbers are measured on CNNs, with CNN→transformer transfer largely unvalidated (NeuSight is a notable exception). **Hardware generalization** shows promise through meta-learning (HELP: 10-sample adaptation), feature-based transfer (LitePred: 85 devices),

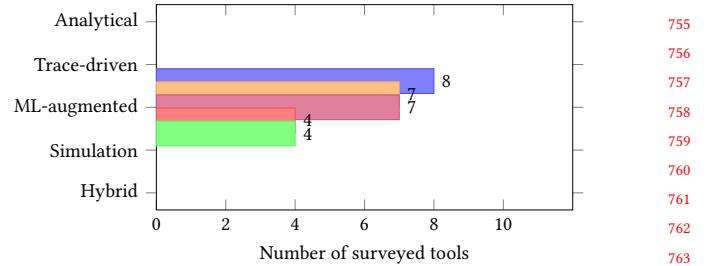


Figure 5: Distribution of surveyed tools by methodology type. Hybrid approaches achieve the best accuracy despite being underrepresented (4 tools).

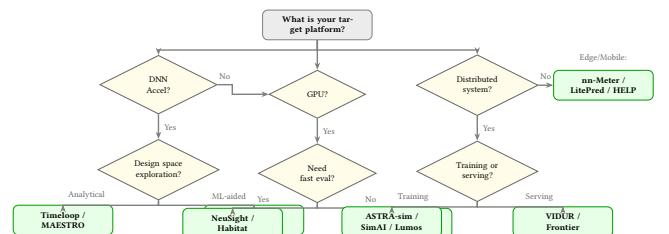


Figure 6: Practitioner decision flowchart for tool selection. Platform determines the candidate set; speed and use case narrow the choice.

and analytical decomposition (Habitat), but cross-family transfer (GPU→TPU→PIM) remains unsolved. **Temporal generalization**—software stack evolution invalidating trained models—is addressed by no surveyed tool.

Analytical models provide actionable design insight: Timeloop identifies data movement bottlenecks, MAESTRO reveals suboptimal dataflows, VIDUR exposes scheduling inefficiencies. ML-augmented approaches offer feature importance but limited causal understanding; hybrid approaches (NeuSight, Concorde) provide partial interpretability. The gap is practically significant: architects need to understand *why* a design is slow, not just predict *that* it is slow.

6.3 Practitioner Tool Selection

Figure 6 presents a decision flowchart for tool selection; Figure 7 plots the speed–accuracy trade-off.

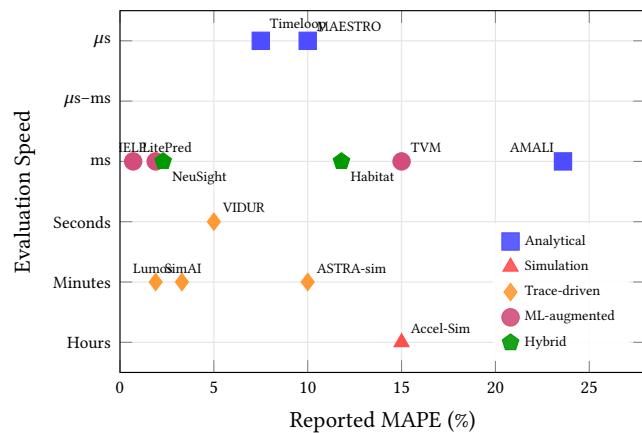
Three recommendations: (1) For *accelerator DSE*, use Timeloop or MAESTRO for microsecond-speed exhaustive search with interpretable bottleneck feedback. (2) For *GPU evaluation*, NeuSight offers the best accuracy–speed balance for LLMs; use Accel-Sim when microarchitectural detail is needed. (3) For *distributed systems*, use VIDUR for LLM serving configuration and ASTRA-sim or SimAI for training parallelism at scale.

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).

Table 4: Comparative analysis of representative tools across key dimensions. Accuracy figures are as reported in original papers; direct comparison is limited by differences in benchmarks, workloads, hardware targets, and evaluation protocols.[†]Unverifiable. ^{*}Surrogate fidelity, not hardware accuracy.

Tool	Methodology	Accuracy (reported)	Setup Cost	Generalization	Interpretability	Eval. Speed
Timeloop [50]	Analytical	5–10%	Arch spec only	Any accelerator	High	μs
MAESTRO [38]	Analytical	5–15%	Arch spec only	Any accelerator	High	μs
AMALI [9]	Analytical	23.6% MAPE	None	GPU LLM inference	High	ms
Accel-Sim [34]	Simulation	10–20%	GPU binary	GPU-specific	High	Hours
ASTRA-sim [71]	Trace-driven	5–15%	Execution trace	Configurable	Medium	Minutes
VIDUR [3]	Trace-driven	<5%	Kernel profiles	LLM-specific	High	Seconds
SimAI [68]	Trace-driven	1.9%	Full-stack setup	LLM training	Medium	Minutes
Lumos [45]	Trace-driven	3.3%	Execution trace	LLM training	Medium	Minutes
nn-Meter [77]	ML-augmented	<1% [†]	1K samples/kernel	Device-specific	Medium	ms
LitePred [16]	ML-augmented	0.7% MAPE	100 samples/device	85+ devices	Low	ms
HELP [41]	ML-augmented	1.9% MAPE	10 samples/device	Cross-platform	Low	ms
TVM [10]	ML-augmented	~15% MAPE	10K+	Operator-level	Medium	ms
NeuSight [42]	Hybrid	2.3% MAPE	Pre-trained	Cross-GPU	Medium	ms
Habitat [75]	Hybrid	11.8% MAPE	Online profiling	Cross-GPU	Medium	Per-kernel
ArchGym [37]	Hybrid	0.61% RMSE*	Simulation runs	Arch-specific	Medium	ms
Concorde [49]	Hybrid	2% CPI	Training corpus	Cross- μ arch	Medium	ms

**Figure 7: Speed-accuracy trade-off. Hybrid approaches (upper-left) achieve fast evaluation and low error; cycle-accurate simulation (lower-right) provides highest fidelity at impractical speeds.**

Environment and rubric. 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 score each tool on a 10-point rubric: *Setup* (3 pts), *Reproducibility* (4 pts), *Usability* (3 pts). Table 5 summarizes results.

7.1 Per-Tool Results

VIDUR (9/10)—the highest-scoring tool. We simulated Llama-2-7B inference on a simulated A100 using vLLM and Sarathi scheduling (Table 6). VIDUR correctly captures scheduling trade-offs: Sarathi achieves 12.2% lower latency than vLLM (0.158 s vs. 0.177 s)

Table 5: Reproducibility evaluation scores (10-point rubric). Tools are ranked by total score. [†]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 6: VIDUR simulation results for Llama-2-7B inference serving on a simulated A100 GPU. All metrics from our own experiments.

Metric	vLLM	Sarathi
Requests	200	50
Avg E2E latency (s)	0.177	0.158
P99 E2E latency (s)	0.320	0.270
Avg TTFT (s)	0.027	0.025
Avg TPOT (s)	0.0093	0.0090
Requests preempted	53	0

via chunked prefill [2], TPOT differs by only 3.5% (confirming hardware-bound decode), and vLLM preempted 26.5% of requests while Sarathi preempted zero—matching the algorithmic difference in KV-cache management [39]. VIDUR’s Docker-pinned dependencies avoid the serialization failures seen in nn-Meter.

Timeloop (9/10). The Docker image provides CLI tools that work correctly for Eyeriss-like configurations with fully deterministic, bit-identical outputs—a significant reproducibility strength. Reference outputs for standard designs (Eyeriss, Simba) enable verification

Table 7: ASTRA-sim quantitative results from our experiments on the HGX-H100 configuration. Top: collective microbenchmarks (8 NPUs, 1MB). 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%

without hardware. However, Python bindings fail (`ImportError: libbarvinok.so.23`), preventing programmatic use.

ASTRA-sim (8.5/10). We executed 8-NPU collective microbenchmarks and ResNet-50 data-parallel training at 2–8 GPUs on HGX-H100 (Table 7). Collective operation ratios are physically plausible: Reduce-Scatter takes half the time of All-Reduce (consistent with half the data), while All-to-All takes ~2× All-Reduce. Communication overhead scales from 0.05% (2 GPUs) to 0.30% (8 GPUs)—a 5.76× increase for 4× more GPUs, consistent with ring All-Reduce scaling. Scale coverage is limited to 8 NPUs by included topology files.

NeuSight (7.5/10). The tile-based decomposition correctly mirrors CUDA tiling for standard dense operations, but testing on irregular workloads was limited by missing examples, suggesting the tool is best validated for regular LLM workloads.

nn-Meter (3/10)—the lowest-scoring tool. After four installation attempts (>4 hours), we could not execute *any* predictions due to a chain of unpinned dependencies: pickle-serialized predictors (scikit-learn 0.23.1) are incompatible with current versions, and onnx-simplifier fails on aarch64. The claimed <1% MAPE is **unverifiable on any current software stack**; the tool has received no updates since 2022.

7.2 Lessons and Threats to Validity

Five lessons emerge: (1) **Docker-first deployment** is the strongest reproducibility predictor—all three Docker-based tools scored 8.5+/10 while nn-Meter scored 3/10. (2) **ML model serialization is fragile**—nn-Meter’s pickle-based storage became unusable within two years; tools should use version-stable formats or provide retraining scripts. (3) **Reference outputs enable trust without hardware**—Timeloop and ASTRA-sim include verifiable reference results. (4) **Scale-limited evaluation understates system tools**—our 2–8 GPU tests show only 0.30% communication overhead, far below production scales [13]. (5) **Reproducible accuracy claims should be weighted higher** than unrepeatable ones, regardless of the claimed number.

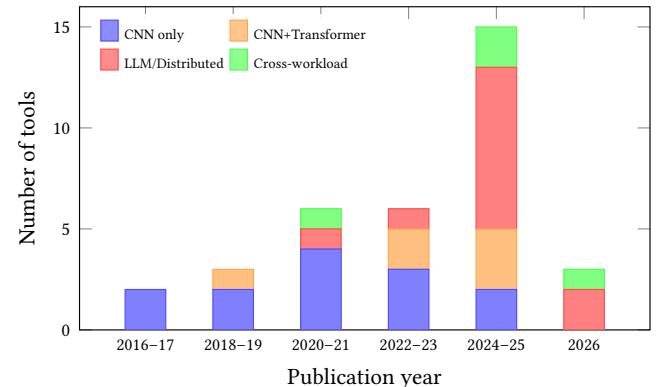


Figure 8: Workload coverage of surveyed tools by publication period. The shift toward transformer and LLM workloads accelerates from 2023, but MoE and diffusion models remain largely uncharacterized.

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

8 Open Challenges and Future Directions

Workload coverage gaps. Existing tools are primarily validated on CNNs; transformers, MoE, diffusion models, and dynamic inference [36] remain underrepresented. Neural scaling laws [12, 20, 24, 33] predict training loss but not hardware-specific latency. Figure 8 shows the shift: before 2022, nearly all tools targeted CNNs; from 2023, LLM workloads increasingly appear, but MoE and diffusion remain uncharacterized.

The composition problem. Composing kernel-level predictions into end-to-end estimates is unsolved. NeuSight achieves 2.3% kernel-level MAPE, but for a 100-layer model, independent errors yield ~10× higher variance ($\sigma_{\text{model}} \approx \sigma_{\text{kernel}} \cdot \sqrt{N}$); correlated errors can compound linearly, potentially yielding 20–30% model-level error. VIDUR sidesteps this by profiling entire prefill/decode phases. Three approaches merit investigation: error propagation analysis, end-to-end calibration, and hierarchical joint prediction across abstraction levels.

Emerging hardware and design integration. PIM architectures [23, 28, 40, 51], chiplets, and disaggregated designs blur conventional memory hierarchy assumptions. Compiler integration needs uncertainty quantification [10, 78]; LLM serving needs real-time prediction; and hardware-aware optimizations (FlashAttention [14]) change the performance landscape faster than models can be retrained.

Reproducibility and trust. While MLPerf [47, 59] standardizes hardware *measurement*, no equivalent exists for performance *prediction*—standardized prediction benchmarks with common workloads and evaluation protocols would significantly advance the field.

Future directions. Five priorities: (1) Transformer/MoE-aware tools with validated non-CNN accuracy; (2) validated composition

1045 methods with bounded end-to-end error; (3) unified energy-latency-
 1046 memory prediction [58]; (4) temporal robustness benchmarks for
 1047 software stack evolution; (5) unified tooling with Docker-first de-
 1048 ployment, portable formats (ONNX), and standard workload repre-
 1049 sentations (Chakra [63]).

1050

1051 9 Conclusion

1052 This survey analyzed over 30 tools for predicting ML workload
 1053 performance, organized by methodology type, target platform, and
 1054 abstraction level. Key findings: (1) *Methodology determines trade-*
 1055 *offs, not quality*—analytical models offer microsecond interpretable
 1056 evaluation, trace-driven simulators provide 2–15% system-level
 1057 error, and hybrid approaches achieve the best accuracy-speed bal-
 1058 ance (NeuSight: 2.3% MAPE). (2) *LLM workloads demand specialized*
 1059 *modeling*—prefill/decode distinctions, KV cache management, and
 1060 dynamic batching require purpose-built tools (VIDUR, Frontier)
 1061 rather than CNN-era extensions. (3) *Reproducibility is a practical*
 1062 *bottleneck*—Docker-first tools score 8.5+/10 while tools relying on
 1063 serialized ML models have become unusable. (4) *Accuracy claims*
 1064 *require scrutiny* due to varying benchmarks and metrics.

1065 The most pressing gaps are CNN-to-transformer generalization,
 1066 kernel-to-end-to-end composition, emerging hardware support
 1067 (PIM, chiplets), and reproducibility failures. As ML workloads grow
 1068 in scale and diversity, this survey provides practitioners guidance
 1069 for tool selection and researchers a roadmap for advancing the field.

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