# MLCommons Science Working Group AI Benchmarks Collection

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#### Abstract

This document provides an overview of various benchmarks, including their descriptions, URLs, domains, focus areas, keywords, task types, AI capabilities measured, metrics, models, and notes. Each benchmark

### Citation

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1 Benchmark Overview Table

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
MMU Massive Multitask Language Understanding) dataset  The ification  metric reference SNALtion downferstation	MMLU (Massive Multitask Language Understanding)	Multidomain	Academic knowl- edge and reasoning across 57 subjects	multitask, multiple- choice, zero-shot, few-shot, knowledge probing	Multiple choice	General reasoning, subject- matter under- standing	Accuracy	GPT-40, Gemini 1.5 Pro, o1, DeepSeek- R1	[1]⇒
reference 364410n douerflentation  Winogrande	CommonSense	ANLP; Commonsense	Commonsens question answering	e ConceptNet, multiple- choice, adver- sarial	Multiple choice	Commonsense reasoning and knowledge integration	Accuracy	BERT- large, RoBERTa, GPT-3	[2]⇒
dataset The file alon metres and the file alon metres and the file alon metres and the file along the file alon	Winogrande	NLP; Commonsense	Winograd Schema- style pronoun resolution	adversarial, pronoun resolution	Pronoun resolu- tion	Robust commonsense reasoning	Accuracy, AUC	RoBERTa, BERT, GPT-2	[3]⇒
BIG-Bench (Beyond the Initiation Game Benchmark) dataset The Initiation Game Benchmark (Basical Games Benchmark) dataset The Initiation Games Benchmark (Beyond Games Benchmark) dataset The Initiation Games Benchmark (Beyond Games Benchmark) dataset (Beyond Games B	BIG-Bench (Beyond the Imita- tion Game Benchmark)	NLP; AI Evaluation	Diverse reasoning and gen- eralization tasks	few-shot, multi-task, bias analysis	Few-shot eval- uation, Multi- task evaluation	Reasoning and generalization across diverse tasks	Accuracy, Task- specific metrics	GPT-3, Dense Transform- ers, Sparse Transform- ers	[4]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
ClimateLearn datase Topic (ration) metric datase Topic (ration) metric datase (ration) metric dataset	··· ClimateLearn	Climate Science; Forecasting	ML for weather and cli- mate modeling	medium- range fore- casting, ERA5, data- driven	Forecasting	Global weather prediction (3-5 days)	RMSE, Anomaly correlation	CNN baselines, ResNet variants	[5]⇒
CFDBench (Fluid Dynamics) datasia Specification metris Specification reference Specific dissemination	CFDBench (Fluid Dy- namics)	Fluid Dy- namics; Scientific ML	Neural operator surrogate modeling	neural oper- ators, CFD, FNO, Deep- ONet	Surrogate modeling	Generalization of neural op- erators for PDEs	L2 error, MAE	FNO, DeepONet, U-Net	[6]⇒
Satinglet dataset Typer(if ation dataset South	SatImgNet	Remote Sensing	Satellite imagery classifica- tion	land-use, zero-shot, multi-task	Image classification	Zero-shot land-use classification	Accuracy	CLIP, BLIP, ALBEF	[7]⇒
Quantum Computing Benchmarks (QML)  datases Specification metrics Specification reference Specification assemblemation	Quantum Computing Benchmarks (QML)	Quantum Computing	Quantum algorithm perfor- mance evaluation	quantum circuits, state prepara- tion, error correction	Circuit benchmarking, State classification	Quantum algorithm performance and fidelity	Fidelity, Success probability	IBM Q, IonQ, AQT@LBNL	[8]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
OCP (Open Catalyst Project)  dalasas  The Preation  metrics  reference buildion downmentation	OCP (Open Catalyst Project)	Chemistry; Materials Science	Catalyst adsorption energy prediction	DFT re- laxations, adsorption energy, graph neural net- works	Energy prediction, Force prediction	Prediction of adsorption energies and forces	MAE (energy), MAE (force)	CGCNN, SchNet, DimeNet++, GemNet- OC	[9]− [12]⇒
metrics Solution Governmentation	$^*$ $^*$ $^*$ $^*$ $^*$ $^*$	Medical Question Answering	Medical board exam QA	USMLE, diagnostic QA, medical knowledge, multilingual	Multiple choice	Medical diagnosis and knowledge retrieval	Accuracy	Neural reader, Retrieval- based QA systems	[13]⇒
Materials Project  datasas — Specification  metrica — Specification  reference Specification — Specification	Materials Project	Materials Science	DFT-based property prediction	DFT, materials genome, high-throughput	Property prediction	Prediction of inorganic material properties	MAE, R^2	Automatmine Crystal Graph Neural Networks	$\operatorname{er}[14] \Rightarrow$
GPQA Diamond datasas Specification metrica Specification metrica Specification generation	GPQA Dia- mond	Science	Graduate- level sci- entific reasoning	Google-proof, graduate- level, science QA, chem- istry, physics	Multiple choice, Multi-step QA	Scientific reasoning, deep knowledge	Accuracy	o1, DeepSeek- R1	[15]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
ARC-Challenge (Advanced Reasoning Challenge)  datases specific stein  metrics software dawners and specific stein  reference shadio dawnerstation	ARC- Challenge (Advanced Reasoning Challenge)	Science	Grade- school science with rea- soning emphasis	grade-school, science QA, challenge set, reasoning	Multiple choice	Commonsense and scientific reasoning	Accuracy	GPT-4, Claude	[16]⇒
Humanity's Last Exam dataset Transcription of the Company of the C	Humanity's Last Exam	Multidomain	Broad cross- domain academic reasoning	cross-domain, academic exam, multiple- choice, multi- disciplinary	Multiple choice	Cross-domain academic rea- soning	Accuracy	unkown	[17]⇒
FrontierMath  datasa  Type (Reation  metr see Souldion desembertation	FrontierMath	Mathematics	Challenging advanced mathe- matical reasoning	symbolic reasoning, number theory, algebraic geometry, category theory	Problem solving	Symbolic and abstract mathe- matical reason- ing	Accuracy	unkown	[18]⇒
reference 364400 specification	SciCode	Scientific Program- ming	Scientific code gener- ation and problem solving	code synthesis, scientific computing, programming benchmark	Coding	Program synthesis, scientific computing	Solve rate (%)	Claude3.5- Sonnet	[19]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
AMME (American invitational Mathematics Examination) Mathematics Examination) datassas  mattris  meterence sessation gasemientation	AIME (American Invitational Mathematics Examination)	Mathematics	Pre-college advanced problem solving	algebra, combinatorics, number theory, geometry	Problem solving	Mathematical problem-solving and reasoning	Accuracy	unkown	[20]⇒
MATH-500  datases  matrix  reference Seaton assementation	MATH-500	Mathematics	Math reasoning generalization	calculus, algebra, number theory, geometry	Problem solving	Math reasoning and generaliza- tion	Accuracy	unkown	[21]⇒
CURIE (Scientific Long-Centext Understanding, Reasoning and Information Extraction)  dataset  metr  reference southing assemination	CURIE (Scientific Long-Context Understanding, Reasoning and Information Extraction)	Multidomain Science	Long-context scientific reasoning	long-context, information extraction, multimodal	Information extraction, Reasoning, Concept tracking, Aggregation, Algebraic manipulation, Multimodal comprehension	Long-context understanding and scientific reasoning	Accuracy	unkown	[22]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
FEABench (Finite Element Analysis Benchmark) dataspa Specification metric South Specification reference South Specification	FEABench (Finite Element Analysis Benchmark)	Computation Engineer- ing	alFEA simulation accuracy and performance	finite element, simulation, PDE	Simulation, Performance evaluation	Numerical simulation accuracy and efficiency	Solve time, Error norm	FEniCS, deal.II	[23]⇒
SPIDA (Scientific Paper Image Question Answering)  datasea Tractication  metric Section (Scientific Section Institution)  reference Section (Scientific Section Institution)	sPIQA (Scientific Paper Image Question Answering)	Computer Science	Multimodal QA on sci- entific figures	multimodal QA, figure understand- ing, table comprehen- sion, chain- of-thought	Question answering, Multimodal QA, Chain- of-Thought evaluation	Visual-textual reasoning in sci- entific contexts	Accuracy, F1 score	Chain-of- Thought models, Multi- modal QA systems	[24]⇒
Baidsench (Biological Al Scientist Benchmark) Scientist Benchmark) datases Specification metrics Specification generation (Bownfernation	BaisBench (Biological AI Scientist Benchmark)	Computation Biology	alOmics- driven AI research tasks	single-cell annotation, biological QA, au- tonomous discovery	Cell type annotation, Multiple choice	Autonomous biological research capabilities	Annotation accuracy, QA accu- racy	LLM-based AI scientist agents	[25]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
MOLGEN datasas Transformation and the second	MOLGEN	Computation Chemistry	alMolecular generation and opti- mization	SELFIES, GAN, property optimization	Distribution learning, Goal- oriented genera- tion	Generation of valid and opti- mized molecular structures	Validity%, Novelty%, QED, Docking score	MolGen	[26]⇒
Open Graph Benchmark (OGB)- Biology datases The (Foaton datases The (Foaton metrics ) Solution	Open Graph Benchmark (OGB) - Biology	Graph ML	Biological graph property prediction	node prediction, link prediction, graph classification	Node property prediction, Link property prediction, Graph property prediction	Scalability and generalization in graph ML for biology	Accuracy, ROC-AUC	GCN, Graph- SAGE, GAT	[27]⇒
JARVIS-Leader-board datases The fination metric solution governmentation	JARVIS- Leaderboard	Materials Science; Bench- marking	Comparative evaluation of materials design methods	leaderboards, materials methods, simulation	Method bench- marking, Leaderboard ranking	Performance comparison across diverse materials design methods	MAE, RMSE, Accuracy	unkown	[28]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
Nixtla Neural Forecast TimeGPT datasia  Topic (Riccion  Topic	Nixtla Neu- ral Forecast TimeGPT	Time- series; General ML	Time-series foundation model "TimeGPT" for forecasting and anomaly detection	TimeGPT, founda- tion model, time-series, generative model	Time-series forecasting, Anomaly detec- tion	Zero-shot forecasting, anomaly detec- tion	RMSE, Anomaly detection metrics	TimeGPT	[29]⇒
Nixtla Neural Forecast NHTS datasas profitation metric selection dataseteristics reference NALIOn dataseteristics	Nixtla Neu- ral Forecast NHITS	Time- series; General ML	Official NHITS imple- mentation for long- horizon time series forecasting	NHITS, long-horizon forecasting, neural in- terpolation, time-series	Time-series fore-casting	Accuracy, compute efficiency for long series	RMSE, MAPE	NHITS	[30]⇒
Nixtla Neural Forecast TimeLLM datases TimeLLM metrics Traference Solution dissemination	Nixtla Neu- ral Forecast TimeLLM	Time- series; General ML	Reprogramm LLMs for time series forecasting	in Fime-LLM, language model, time- series, repro- gramming	Time-series fore-casting	Model reuse via LLM, few-shot forecasting	RMSE, MAPE	Time-LLM	[31]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
Nixta NeuralForceast datasal specification metric solution dissertentation	Nixtla Neu- ralForecast	Time- series fore- casting; General ML	High- performance neural fore- casting library with >30 models	time-series, neural fore- casting, NBEATS, NHITS, TFT, probabilistic forecasting, usability	Time-series fore-casting	Forecast accuracy, interpretability, speed	RMSE, MAPE, CRPS	NBEATS, NHITS, TFT, DeepAR	[32]⇒
vLLM Performance Dashboard dataset metric dataset reference 3-button gasententation	vLLM Perfor- mance Dash- board	LLM; HPC/inferen	Interactive cedashboard showing inference perfor- mance of vLLM	Dashboard, Throughput visualization, Latency anal- ysis, Metric tracking	Performance visualization	Throughput, latency, hardware utilization	Tokens/sec, TTFT, Memory usage	LLaMA-2, Mistral, Qwen	[33]⇒
vLLM inference and Serving Engine Engine Engine datases Topocification reference Solution governmentation	vLLM In- ference and Serving En- gine	LLM; HPC/inferen	High- cethroughput, memory- efficient inference and serving engine for LLMs	LLM inference, Page-dAttention, CUDA graph, streaming API, quantization	Inference Bench- marking	Throughput, latency, memory efficiency	Tokens/sec, Time to First Token (TTFT), Memory footprint	LLaMA, Mixtral, FlashAttentic based models	

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
Sclang Framework datases specification metric datases specification metric datases specification dataset speci	SGLang Framework	LLM Vision	Fast serving framework for LLMs and visionlanguage models	LLM serving, vision-language, RadixAttention, performance, JSON decoding	Model serving framework	Serving throughput, JSON/task- specific latency	Tokens/sec, Time-to- first-token, Through- put gain vs baseline	LLaVA, DeepSeek, Llama	[35]⇒
jet Classification dataset specification metric solution dissententation	Jet Classification	Particle Physics	Real-time classifi- cation of particle jets using HL-LHC simulation features	classification, real-time ML, jet tagging, QKeras	Classification	Real-time inference, model compression performance	Accuracy, AUC	Keras DNN, QKeras quantized DNN	[36]⇒
regular Sensor Data Compression Compression data season of the Compression data season of the Compression of	Irregular Sensor Data Compression	Particle Physics	Real-time compression of sparse sensor data with autoencoders	compression, autoencoder, sparse data, irregular sampling	Compression	Reconstruction quality, com- pression effi- ciency	MSE, Compression ratio	Autoencoder Quantized autoen- coder	, [37]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
Beam Control dataset specification metric solution deservation deservation deservation	Beam Control	Accelerators and Mag- nets	Reinforcemer learning control of accelera- tor beam position	at RL, beam stabiliza- tion, control systems, simulation	Control	Policy performance in simulated accelerator control	Stability, Control loss	DDPG, PPO (planned)	[38], [39]⇒
Ultrafast jet classification at the HLLHC the HLLHC dataseas Tracification Tracificati	Ultrafast jet classifica- tion at the HL-LHC	Particle Physics	FPGA- optimized real-time jet origin classifica- tion at the HL-LHC	jet classifica- tion, FPGA, quantization- aware train- ing, Deep Sets, In- teraction Networks	Classification	Real-time inference under FPGA constraints	Accuracy, Latency, Resource utilization	MLP, Deep Sets, Inter- action Net- work	[40]⇒
Quench detection datases Truc (Radion metria Truc (Radion) reference 3-skdion Speedmentation	Quench de- tection	Accelerators and Mag- nets	Real-time detection of superconducting magnet quenches using ML	quench detection, autoencoder, anomaly detection, real-time	Anomaly detection, Quench localization	Real-time anomaly de- tection with multi-modal sensors	ROC- AUC, Detection latency	Autoencoder RL agents (in devel- opment)	

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
Intelligent experiments through real-time Al datasets Transformed Al datasets	Intelligent experiments through real-time AI	Instrumentat and De- tectors; Nuclear Physics; Particle Physics	ioReal-time FPGA- based trigger- ing and detector control for sPHENIX and future EIC	FPGA, Graph Neural Network, hls4ml, real- time infer- ence, detector control	Trigger classifi- cation, Detector control, Real- time inference	Low-latency GNN inference on FPGA	Accuracy (charm and beauty detection), Latency (micros), Resource utilization (LUT/FF/B)	Bipartite Graph Net- work with Set Trans- formers (BGN-ST), GarNet (edge- RAMASINGP))	[42]⇒
Neural Architecture Codesign for Pass Physics Applications for Pass Physics Applications datapas 35pc(fication datapas 35pc(fication datapas 35pc(fication datapas 35pc(fication datapas 35pc(fication datapas 35pc)) and passed fication datapas 35pc(fication datapas 35pc) and passed fication datapas 35pc(fication datapas 35pc) and passed fication	Neural Ar- chitecture Codesign for Fast Physics Applications	Physics; Materials Science; Particle Physics	Automated neural ar- chitecture search and hardware- efficient model codesign for fast physics ap- plications	neural architecture search, FPGA deployment, quantization, pruning, hls4ml	Classification, Peak finding	Hardware- aware model optimization; low-latency inference	Accuracy, Latency, Resource utilization	NAC- based BraggNN, NAC- optimized Deep Sets (jet)	[43]⇒
Smart Pixels for LHC dataset  metric reference 364don dissementation	Smart Pixels for LHC	Particle Physics; Instrumen- tation and Detectors	On-sensor, in-pixel ML fil- tering for high-rate LHC pixel detectors	smart pixel, on-sensor in- ference, data reduction, trigger	Image Classification, Data filtering	On-chip, low-power inference; data reduction	Data rejection rate, Power per pixel	2-layer pixel NN	[44]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
HEDM (BraggNN) disasts reference Skillon agamentation	HEDM (BraggNN)	Material Science	Fast Bragg peak anal- ysis using deep learn- ing in diffraction microscopy	BraggNN, diffraction, peak finding, HEDM	Peak detection	High- throughput peak localiza- tion	Localization accuracy, Inference time	${\it BraggNN}$	[45]⇒
aD-STEM datases methys services reference solution desambentation	4D-STEM	Material Science	Real-time ML for scanning trans- mission electron microscopy	4D-STEM, electron mi- croscopy, real-time, image pro- cessing	Image Classification, Streamed data inference	Real-time large- scale microscopy inference	Classification accuracy, Through- put	CNN models (prototype)	[46]⇒
In-Situ High-Speed Computer Vision Wision Section distant Section distant Section Sec	In-Situ High- Speed Com- puter Vision	Fusion/Plasm	naReal-time image clas- sification for in-situ plasma diagnostics	plasma, insitu vision, real-time ML	Image Classification	Real-time diagnostic inference	Accuracy, FPS	CNN	[47]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
BenchGounci Albench datasi  matrix  reference solution gizerfiertation	BenchCouncil AIBench	General	End-to-end AI bench- marking across micro, compo- nent, and application levels	benchmarking, AI systems, application- level evalua- tion	Training, Inference, Endto-end AI workloads	System-level AI workload perfor- mance	Throughput, Latency, Accuracy	ResNet, BERT, GANs, Recom- mendation systems	[48]⇒
BenchCouncil BigDataBench datasas "Specification datasas "Specification metrics" solution reference Specification dissententiation	BenchCouncil Big- DataBench	General	Big data and AI bench- marking across structured, semi- structured, and un- structured data work- loads	big data, AI benchmark- ing, data analytics	Data pre- processing, Inference, End- to-end data pipelines	Data processing and AI model inference perfor- mance at scale	Data through- put, La- tency, Accuracy	CNN, LSTM, SVM, XGBoost	[49]⇒
MLPerf HPC datase Specification metric Soldion discernination	MLPerf HPC	Cosmology, Climate, Protein Structure, Catalysis	Scientific ML training and inference on HPC systems	HPC, training, inference, scientific ML	Training, Inference	Scaling efficiency, training time, model accuracy on HPC	Training time, Accu- racy, GPU utilization	CosmoFlow, DeepCAM, OpenCata- lyst	[50]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
MLCommons Science dataset  metrics  reference Science age-with a service and a service age-with a service and a service age-with a service age-wit	MLCommons Science	Earthquake, Satellite Image, Drug Discovery, Electron Microscope, CFD	AI benchmarks for scientific applications including time-series, imaging, and simulation	science AI, benchmark, MLCom- mons, HPC	Time-series analysis, Image classification, Simulation sur- rogate modeling	Inference accuracy, simulation speed-up, generalization	MAE, Accuracy, Speedup vs simulation	CNN, GNN, Trans- former	[51]⇒
LHC New Physics Dataset dataset  dataset  metres reference solution documentation	LHC New Physics Dataset	Particle Physics; Real-time Triggering	Real-time LHC event filtering for anomaly detec- tion using proton collision data	anomaly detection, proton collision, real-time inference, event filtering, unsupervised ML	Anomaly detection, Event classification	Unsupervised signal detection under latency and bandwidth constraints	ROC- AUC, Detection efficiency	Autoencoder Variational autoen- coder, Isolation forest	, [52]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
MLCommons Medical Al dataset specification metrics seems and a specification metrics seems and a specification of the seems of the seem	MLCommons Medical AI	Healthcare; Medical AI	Federated bench- marking and eval- uation of medical AI mod- els across diverse real-world clinical data	medical AI, federated evaluation, privacy-preserving, fairness, healthcare benchmarks	Federated evaluation, Model validation	Clinical accuracy, fairness, generalizability, privacy compliance	ROC AUC, Accuracy, Fairness metrics	MedPerf- validated CNNs, GaNDLF workflows	[53]⇒
CaloChallenge 2022  dataset Type:(firation  matters	CaloChallenge 2022	LHC Calorime- ter; Parti- cle Physics	Fast generative- model- based calorimeter shower simulation evaluation	calorimeter simulation, generative models, surrogate modeling, LHC, fast simulation	Surrogate modeling	Simulation fi- delity, speed, efficiency	Histogram similarity, Classifier AUC, Gen- eration latency	VAE variants, GAN variants, Normalizing flows, Diffusion models	[54]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
Papers With Code (SOTX Platform) dataset  reference Southon governmentation	Papers With Code (SOTA Platform)	General ML; All domains	Open platform tracking state-of- the-art results, bench- marks, and implemen- tations across ML tasks and papers	leaderboard, benchmark- ing, repro- ducibility, open-source	Multiple (Classification, Detection, NLP, etc.)	Model performance across tasks (accuracy, F1, BLEU, etc.)	Task- specific (Accuracy, F1, BLEU, etc.)	All published models with code	[55]⇒
Codabench datasea pacification metrics reference solution governmentation	Codabench	General ML; Multi- ple	Opensource platform for organizing reproducible AI benchmarks and competitions	benchmark platform, code sub- mission, competi- tions, meta- benchmark	Multiple	Model reproducibility, performance across datasets	Submission count, Leader- board ranking, Task- specific metrics	Arbitrary code submissions	[56]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
Sabath (SB-FAR) dataget  Specification  metric  reference Specific accordination	Sabath (SBI-FAIR)	Systems; Metadata	FAIR metadata frame- work for ML-driven surrogate workflows in HPC systems	meta- benchmark, metadata, HPC, surro- gate modeling	Systems benchmarking	Metadata tracking, repro- ducible HPC workflows	Metadata complete- ness, FAIR compliance	NA	[57]⇒
PDEBench datasal specification metries datasal specification reference solution downternation	PDEBench	CFD; Weather Modeling	Benchmark suite for ML-based surrogates solving time- dependent PDEs	PDEs, CFD, scientific ML, surrogate modeling, NeurIPS	Supervised Learning	Time-dependent PDE model- ing; physical accuracy	RMSE, boundary RMSE, Fourier RMSE	FNO, U- Net, PINN, Gradient- Based inverse methods	[58]⇒
LUM-inference-Bench dataset specification metric solution against action of the second	LLM- Inference- Bench	LLM; HPC/inferen	Hardware ceperfor- mance bench- marking of LLMs on AI acceler- ators	LLM, inference benchmarking, GPU, accelerator, throughput	Inference Bench- marking	Inference throughput, latency, hard- ware utilization	Token throughput (tok/s), Latency, Framework- hardware mix perfor- mance	LLaMA- 2-7B, LLaMA- 2-70B, Mistral-7B, Qwen-7B	[59]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
Delta Squared-DFT dataset The Traction metro.  reference thation governmentation	Delta Squared- DFT	Computation Chemistry; Materials Science	nalBenchmarkin machine- learning corrections to DFT using Delta Squared- trained models for reaction energies	g density functional theory, Delta Squared-ML correction, reaction energetics, quantum chemistry	Regression	High-accuracy energy pre- diction, DFT correction	Mean Absolute Error (eV), Energy ranking accuracy	Delta Squared- ML cor- rection networks, Kernel ridge re- gression	[60]⇒
Uban Data Layer (UDL)  dataset The incidion  metrics  reference 3-skilon downfentation	Urban Data Layer (UDL)	Urban Comput- ing; Data Engineer- ing	Unified data pipeline for multimodal urban science research	data pipeline, urban science, multi-modal, benchmark	Prediction, Classification	Multi-modal urban inference, standardization	Task- specific accuracy or RMSE	Baseline regres- sion/classific pipelines	[61]⇒
LLMs for Crop Science dataset the file atom metrics reference solution governmentation	* LLMs for Crop Science	Agricultural Science; NLP	Evaluating LLMs on crop trait QA and textual inference tasks with domain- specific prompts	crop science, prompt engineering, domain adaptation, question answering	Question Answering, Inference	Scientific knowledge, crop reasoning	Accuracy, F1 score	GPT-4, LLaMA- 2-13B, T5-XXL	[62]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
datasset The fication dataset reference and done done dataset reference and done done done done done done done do	* DUNE	Particle Physics	Real-time ML for DUNE DAQ time-series data	DUNE, time-series, real-time, trigger	Trigger selection, Timeseries anomaly detection	Low-latency event detection	Detection efficiency, Latency	CNN, LSTM (planned)	[63]⇒
MassSpecCym  dataset Spec(Fcation  metrics  reference Solution documentation	MassSpecGym	Cheminforma Molecular Discovery	atiBenchmark suite for discovery and identi- fication of molecules via MS/MS	mass spectrometry, molecular structure, de novo generation, retrieval, dataset	De novo generation, Retrieval, Simulation	Molecular identification and generation from spectral data	Structure accuracy, Retrieval precision, Simulation MSE	Graph- based generative models, Retrieval baselines	[64]⇒
HDR Mi, Anomaly Challenge (Gravitational Waves) discontinuous discontinu	* HDR ML Anomaly Challenge (Gravita- tional Waves)	Astrophysics: Time-series	Detecting anomalous gravitational- wave sig- nals from LIGO/Virgo datasets	anomaly detection, gravitational waves, as- trophysics, time-series	Anomaly detection	Novel event detection in physical signals	ROC- AUC, Preci- sion/Recall	Deep latent CNNs, Au- toencoders	[65]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
HDR ML Anomaly Challenge (Butterfly) datasate page (fication page (fication page)) metrics page (fication page) reference page (fication fication f	HDR ML Anomaly Challenge (Butterfly)	Genomics; Image/CV	Detecting hybrid butterflies via image anomaly detection in genomic- informed dataset	anomaly detection, computer vision, genomics, butterfly hybrids	Anomaly detection	Hybrid detection in biological systems	Classification accuracy, F1 score	CNN- based detectors	[66]⇒
HDR ML Anomaly Challenge (Sea Level Rise) datasea Teed Rise) metrifis September (Sea Level Rise) reference 3-skillion (Sourmentation	HDR ML Anomaly Challenge (Sea Level Rise)	Climate Science; Time- series, Image/CV	Detecting anomalous sea-level rise and flooding events via time- series and satellite imagery	anomaly detection, climate sci- ence, sea-level rise, time- series, remote sensing	Anomaly detection	Detection of environmental anomalies	ROC- AUC, Preci- sion/Recall	CNNs, RNNs, Transform- ers	[67]⇒
Single Qubit Readout on QICK System  dataset System Gradion  metrics Solution documentation	Single Qubit Readout on QICK System	Quantum Computing	Real-time single- qubit state classifica- tion using FPGA firmware	qubit read- out, hls4ml, FPGA, QICK	Classification	Single-shot fi- delity, inference latency	Accuracy, Latency	hls4ml quantized NN	[68]⇒

D - 45	Name	Domain	Focus	IZ		AT C 1-:1:4	Metrics	Models	Citation
Ratings  GPQA: A Graduate-Level Google- Proof Question and Answer	Name	Domain	rocus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
Benchmark  dataset The fredor  reference sauto governmentation	GPQA: A Graduate- Level Google- Proof Ques- tion and Answer Benchmark	Science (Biology, Physics, Chemistry)	Graduate-level, expert- validated multiple- choice questions hard even with web access	Google-proof, multiple- choice, expert reasoning, science QA	Multiple choice	Scientific reasoning, knowledge probing	Accuracy	GPT-4 baseline	[69]⇒
SeafloorAl dataset fination metrics solver s	* SeafloorAI	Marine Science; Vision- Language	Large-scale vision- language dataset for seafloor mapping and ge- ological classifica- tion	sonar imagery, vision- language, seafloor mapping, segmentation, QA	Image segmentation, Visionlanguage QA	Geospatial understanding, multimodal reasoning	Segmentation pixel accu- racy, QA accuracy	SegFormer, ViLT-style multi- modal models	[70]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
SuperCon30  datasi sprinceton  metries solution dissententation	SuperCon3D	Materials Science; Supercon- ductivity	Dataset and models for predict- ing and generating high-Tc supercon- ductors using 3D crystal structures	superconductiv crystal struc- tures, equiv- ariant GNN, generative models	ityRegression (Tc prediction), Generative modeling	Structure-to- property predic- tion, structure generation	MAE (Tc), Validity of generated structures	SODNet, DiffCSP- SC	[71]⇒
GeSS  datasas  metric  reference 3-44tion desembertation	GeSS	Scientific ML; Ge- ometric Deep Learning	Benchmark suite eval- uating geometric deep learn- ing models under real-world distribu- tion shifts	geometric deep learning, distribution shift, OOD robustness, scientific applications	Classification, Regression	OOD performance in scientific settings	Accuracy, RMSE, OOD ro- bustness delta	GCN, EGNN, DimeNet++	[72]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
Vocal Call Locator (VCL)  dataset The (Tradion  metrics  reference 3-station documentation	Vocal Call Locator (VCL)	Neuroscience Bioacous- tics	; Benchmarkin sound-source localization of rodent vocalizations from multichannel audio	g source lo- calization, bioacoustics, time-series, SSL	Sound source localization	Source localization accuracy in bioacoustic settings	Localization error (cm), Re- call/Precision	CNN- based SSL models	[73]⇒
SPIQA (LLM) datasas— peufication metris reference 3-sulton	SPIQA (LLM)	Multimodal Scientific QA; Com- puter Vision	Evaluating LLMs on image- based scientific paper figure QA tasks (LLM Adapter perfor- mance)	multimodal QA, scientific figures, image+text, chain-of-thought prompting	Multimodal QA	Visual reasoning, scientific figure understanding	Accuracy, F1 score	LLaVA, MiniGPT- 4, Owl- LLM adapter variants	[74]⇒

Ratings	Name	Domain	Focus	Keywords	Task Types	AI Capability	Metrics	Models	Citation
The Well dataset The Treation of the Treation	The Well	biological systems, fluid dy- namics, acoustic scattering, astro- physical MHD	Foundation model + surrogate dataset spanning 16 physical simulation domains	surrogate modeling, founda- tion model, physics sim- ulations, spatiotempo- ral dynamics	Supervised Learning	Surrogate modeling, physics-based prediction	Dataset size, Do- main breadth	FNO baselines, U-Net baselines	[75]⇒

## 2 Radar Chart Table

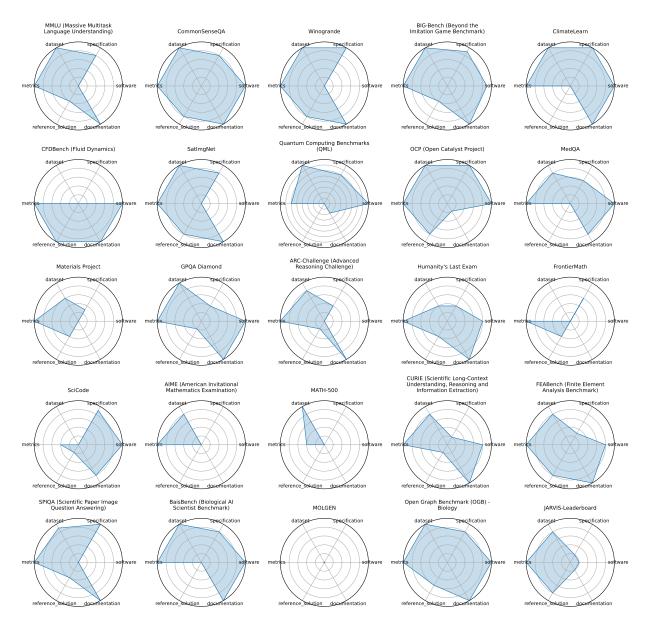


Figure 1: Radar chart overview (page 1)

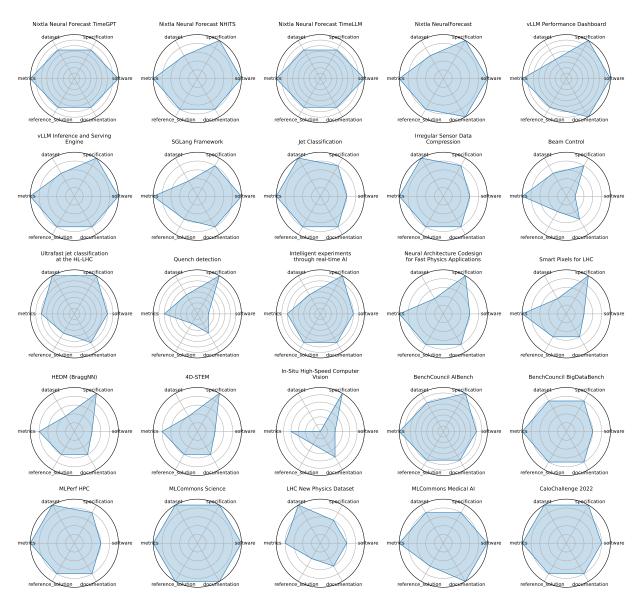


Figure 2: Radar chart overview (page 2)

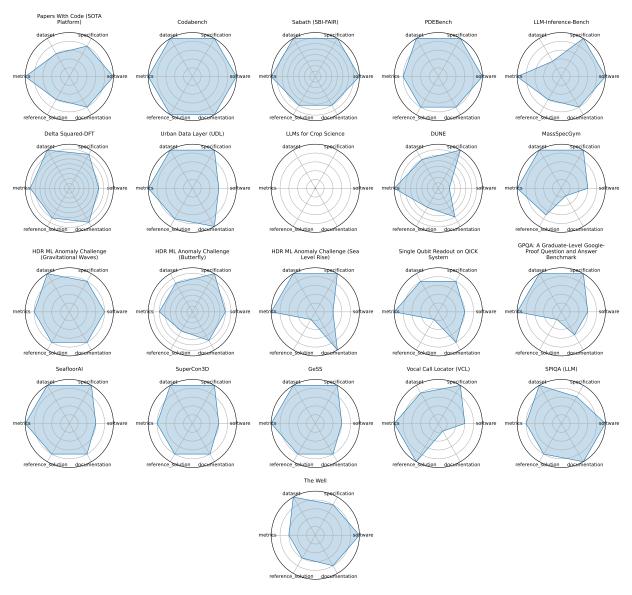


Figure 3: Radar chart overview (page 3)

## 3 Benchmark Details

## 3.1 MMLU (Massive Multitask Language Understanding)

Measuring Massive Multitask Language Understanding (MMLU) is a benchmark of 57 multiple-choice tasks covering elementary mathematics, US history, computer science, law, and more, designed to evaluate a model's breadth and depth of knowledge in zero-shot and few-shot settings.

date: 2020-09-07

version:

 last\_updated:
 2020-09-07

 expired:
 false

 valid:
 yes

 valid date:
 2025-07-28

url: https://paperswithcode.com/dataset/mmlu

doi: 10.48550/arXiv.2009.03300

domain: Multidomain

focus: Academic knowledge and reasoning across 57 subjects

keywords: - multitask - multiple-choice - zero-shot - few-shot - knowledge probing

licensing: MIT License task\_types: - Multiple choice

ai\_capability\_measured: - General reasoning, subject-matter understanding

metrics: - Accuracy

models: - GPT-4o - Gemini 1.5 Pro - o1 - DeepSeek-R1

 $ml\_motif:$  - General knowledge

type: Benchmark

ml task: - Supervised Learning

solutions: 1 notes: Good

contact.name: Dan Hendrycks contact.email: dan (at) safe.ai

datasets.links.name: Papers with Code datasets

datasets.links.url: https://github.com/paperswithcode/paperswithcode-data

results.links.name: Chinchilla

results.links.url: https://arxiv.org/abs/2203.15556

fair.reproducible: True fair.benchmark ready: True

d: mmlu massive multitask language understanding

Citations: [1]

#### Ratings:

Rating	Value	Reason
dataset	5	Meets all FAIR principles and properly versioned.
documentation	5	Well-explained in a provided paper.
metrics	5	Fully defined, represents a solution's performance.
reference solution	2	Reference models are available (i.e. GPT-3), but are not trainable or publicly documented
software	0	No instructions to download or run data given on the site
specification	4	No system constraints

MMLU (Massive Multitask Language Understanding)



### 3.2 CommonSenseQA

CommonsenseQA is a challenging multiple-choice QA dataset built from ConceptNet, requiring models to apply commonsense knowledge to select the correct answer among five choices.

date: 2019-11-20

version:

 last\_updated:
 2019-11-20

 expired:
 false

 valid:
 yes

 valid date:
 2019-11-20

 ${\bf url:} \hspace{1.5cm} {\bf https://paperswithcode.com/paper/commonsenseqa-a-question-answering-challenge}$ 

**doi:** 10.48550/arXiv.1811.00937

domain: NLP; Commonsense

focus: Commonsense question answering

keywords: - ConceptNet - multiple-choice - adversarial

licensing: MIT

task types: - Multiple choice

ai capability measured: - Commonsense reasoning and knowledge integration

metrics: - Accuracy

models:
- BERT-large - RoBERTa - GPT-3
ml\_motif:
- Commonsense question answering

type: Benchmark

ml task: - Supervised Learning

solutions: 2

notes: Baseline 56%, human 89%

contact.name: Alon Talmor, Jonathan Herzig, Nicholas Lourie, Jonathan Berant

contact.email: Unknown

datasets.links.name: CommonsenseQA Dataset (Hugging Face)

datasets.links.url: https://huggingface.co/datasets/commonsense\_qa
results.links.name: Papers With Code Leaderboard for CommonsenseQA
results.links.url: https://paperswithcode.com/dataset/commonsenseqa

fair.reproducible: True fair.benchmark ready: True

id: commonsenseqa

Citations: [2]

#### Ratings:

Rating	Value	Reason
dataset	5	Public, versioned, and FAIR-compliant; includes metadata, splits, and licensing; well-
		integrated with HuggingFace and other ML libraries.
documentation	5	Given in paper.
metrics	5	Accuracy is a simple, reproducible metric aligned with task goals; no ambiguity in evaluation.
$reference\_solution$	4	Several baseline models (e.g., BERT, RoBERTa) are reported with scores; implementations exist in public repos, but not run with hardware constraints
software	5	All code given on Github site
specification	4	Task and format (multiple-choice QA with 5 options) are clearly defined; grounded in
		ConceptNet with consistent structure, though no hardware/system constraints are spec-
		ified.



## 3.3 Winogrande

WinoGrande is a large-scale adversarial dataset of 44,000 Winograd Schema-style questions with reduced bias using AFLite, serving as both a benchmark and transfer learning resource.

date: 2019-07-24

version:

 last\_updated:
 2019-07-24

 expired:
 false

 valid:
 yes

 valid date:
 2019-07-24

 ${\bf url:} \hspace{1.5cm} {\bf https://leaderboard.allenai.org/winogrande/submissions/public}$ 

doi: 10.48550/arXiv.1907.10641

domain: NLP; Commonsense

focus: Winograd Schema-style pronoun resolution

keywords: - adversarial - pronoun resolution

licensing: CC-BY

task types: - Pronoun resolution

ai capability measured: - Robust commonsense reasoning

metrics: - Accuracy - AUC

models:
- RoBERTa - BERT - GPT-2
ml motif:
- Commonsense reasoning

type: Benchmark

ml task: - Supervised Learning

solutions: 2

notes: Human ~94%
contact.name: Keisuke Sakaguchi
contact.email: keisukes@allenai.org
datasets.links.name: Hugging Face / AllenAI

datasets.links.url: https://huggingface.co/datasets/allenai/winogrande

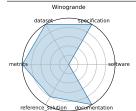
results.links.name: Papers With Code leaderboard

results.links.url: https://paperswithcode.com/dataset/winogrande

fair.reproducible: True
fair.benchmark\_ready: True
id: winogrande
Citations: [3]

Ratings:

Rating	Value	Reason
dataset	5	Public, versioned, and FAIR-compliant with AFLite-generated splits to reduce annotation
		artifacts; hosted by AllenAI with good metadata.
documentation	5	Dataset page and paper provide sufficient detail
metrics	5	Accuracy and AUC are quantitative and well-aligned with disambiguation goals; stan-
		dardized across evaluations.
reference_solution	4	Baseline results available, requiring users to submit their methods along with their sub-
_		missions. Constraints are not required in submissions.
software	0	No template code provided
specification	5	Task (pronoun/coreference resolution) is clearly defined in Winograd Schema style, with
		consistent input/output format; no system constraints included.



## 3.4 BIG-Bench (Beyond the Imitation Game Benchmark)

BIG-Bench is a collaborative suite of 204 tasks designed to probe LLMs' reasoning, knowledge, and bias across diverse domains and difficulty levels beyond simple imitation.

date: 2022-06-09

version:

 last\_updated:
 2022-06-09

 expired:
 false

 valid:
 yes

 valid date:
 2022-06-09

url: https://github.com/google/BIG-bench

 doi:
 10.48550/arXiv.2206.04615

 domain:
 NLP; AI Evaluation

focus: Diverse reasoning and generalization tasks keywords: - few-shot - multi-task - bias analysis

licensing: Apache-2.0

task\_types:
Few-shot evaluation - Multi-task evaluation
ai capability measured:
Reasoning and generalization across diverse tasks

metrics: - Accuracy - Task-specific metrics

models: - GPT-3 - Dense Transformers - Sparse Transformers

ml\_motif: - LLM evaluation type: Benchmark

ml task: - Supervised Learning

solutions: Multiple, including human baselines

notes:Human baselines includedcontact.name:Aarohi Srivastava et al.contact.email:bigbench@googlegroups.com

datasets.links.name: BIG-Bench GitHub Repository (contains tasks and data)

datasets.links.url: https://github.com/google/BIG-bench/tree/main/bigbench/benchmark tasks

results.links.name: BIG-Bench GitHub Repository (results in papers and code)

results.links.url: https://github.com/google/BIG-bench

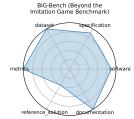
fair.reproducible: True fair.benchmark ready: True

id: big-bench\_beyond\_the\_imitation\_game\_benchmark

Citations: [4]

#### Ratings:

Rating	Value	Reason
dataset	5	Public, versioned, and well-documented; FAIR overall
documentation	5	Explained in the associated paper.
metrics	5	Many tasks use standard quantitative metrics (accuracy, BLEU, F1). Others involve subjective ratings (e.g., Likert), which reduces cross-task comparability.
${\tt reference\_solution}$	2	Human baselines and LLM performance results are included; however, runnable reference solutions are limited and setup is not fully turnkey.
software	4.5	Quick start notebook provided, but instructions on how to run it are lacking.
specification	4.5	Tasks are diverse and clearly described; input/output formats are usually defined but vary widely, and system constraints are not standardized.



# 3.5 ClimateLearn

ClimateLearn provides standardized datasets and evaluation protocols for machine learning models in medium-range weather and climate forecasting using ERA5 reanalysis.

date: 2023-07-19

version:

 last\_updated:
 2023-07-19

 expired:
 false

 valid:
 yes

 valid date:
 2023-07-19

 url:
 https://arxiv.org/abs/2307.01909

 doi:
 10.48550/arXiv.2307.01909

 domain:
 Climate Science; Forecasting

focus: ML for weather and climate modeling

**keywords:** - medium-range forecasting - ERA5 - data-driven

licensing: CC-BY-4.0 task types: - Forecasting

 ai\_capability\_measured:
 - Global weather prediction (3-5 days)

 metrics:
 - RMSE - Anomaly correlation

 models:
 - CNN baselines - ResNet variants

 ml motif:
 - Forecasting - Benchmarking

type: Benchmark

ml task: - Supervised Learning

solutions: Multiple baseline models provided notes: Includes physical and ML baselines.

contact.name: Jason Jewik

contact.email: jason.jewik@ucla.edu

datasets.links.name: ClimateLearn GitHub Repository (data loaders and processing)

datasets.links.url: https://github.com/aditya-grover/climate-learn

results.links.name: ClimateLearn Paper (results section) results.links.url: https://arxiv.org/abs/2307.01909

fair.reproducible: True
fair.benchmark\_ready: True
id: Climatelearn

Citations: [5]

Rating	Value	Reason
dataset	5	Provides standardized access to ERA5 and other reanalysis datasets, with ML-ready
		splits, metadata, and Xarray-compatible formats; versioned and fully FAIR-compliant.
documentation	5	Explained in the benchmark's paper.
metrics	5	ACC and RMSE are standard, quantitative, and appropriate for climate forecasting; well-
		integrated into the benchmark, though interpretation across domains may vary.
reference solution	0	The benchmark is geared for CNN architectures, but no specific model was mentioned.
software	5	Quickstart notebook makes for easy usage
specification	5	Task framing (medium-range climate forecasting), input/output formats, and evaluation
		windows are clearly defined; benchmark supports both physical and learned models with
		detailed constraints.



# 3.6 CFDBench (Fluid Dynamics)

CFDBench provides large-scale CFD data for four canonical fluid flow problems, assessing neural operators' ability to generalize to unseen PDE parameters and domains.

date: 2024-10-01

version:

 last\_updated:
 2024-10-01

 expired:
 false

 valid:
 yes

 valid\_date:
 2024-10-01

url: https://arxiv.org/abs/2310.05963
doi: 10.48550/arXiv.2310.05963
domain: Fluid Dynamics; Scientific ML
focus: Neural operator surrogate modeling

keywords: - neural operators - CFD - FNO - DeepONet

licensing: CC-BY-4.0

task types: - Surrogate modeling

ai capability measured: - Generalization of neural operators for PDEs

metrics: - L2 error - MAE

models: - FNO - DeepONet - U-Net

ml\_motif:
- Generalization
type:
Benchmark

ml task: - Supervised Learning

solutions: Numerous, as it's a benchmark for ML models

notes: 302K frames across 739 cases

contact.name: Yining Luo

contact.email: yining.luo@mail.utoronto.ca

datasets.links.name:unknowndatasets.links.url:unknownresults.links.name:unknownresults.links.url:unknownfair.reproducible:Truefair.benchmarkready:

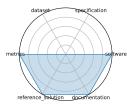
id: cfdbench\_fluid\_dynamics

Citations: [6]

#### Ratings:

Rating	Value	Reason
dataset	0	Not given
documentation	5	Associated paper gives all necessary information.
metrics	5	Quantitative metrics (L2 error, MAE, relative error) are clearly defined and align with regression task objectives.
reference solution	5	Baseline models like FNO and DeepONet are implemented, hardware specified.
software	5	The benchmark provides Python scripts for data loading, preprocessing, and model training/evaluation
specification	0	Not listed

CFDBench (Fluid Dynamics)



# 3.7 SatImgNet

SATIN (sometimes referred to as SatImgNet) is a multi-task metadataset of 27 satellite imagery classification datasets evaluating zero-shot transfer of vision-language models across diverse remote sensing tasks.

date: 2023-04-23

version:

 last\_updated:
 2023-04-23

 expired:
 false

 valid:
 yes

 valid date:
 2023-04-23

url: https://huggingface.co/datasets/saral-ai/satimagnet

doi: 10.48550/arXiv.2304.11619

domain: Remote Sensing

focus: Satellite imagery classification keywords: - land-use - zero-shot - multi-task

licensing: CC-BY-4.0

task types: - Image classification

ai capability measured: - Zero-shot land-use classification

metrics: - Accuracy

models: - CLIP - BLIP - ALBEF
ml\_motif: - Transfer Learning

type: Benchmark

ml task: - Supervised Learning

solutions: Numerous, evaluated via leaderboard

notes: Public leaderboard available

contact.name:Jonathan Robertscontact.email:j.roberts@cs.ox.ac.ukdatasets.links.name:SatImgNet on Hugging Face

datasets.links.url: https://huggingface.co/datasets/saral-ai/satimagnet

results.links.name: SatImgNet Leaderboard

results.links.url: https://huggingface.co/spaces/saral-ai/satin-leaderboard

fair.reproducible: True
fair.benchmark\_ready: True
id: satingnet
Citations: [7]

Rating	Value	Reason
dataset	5	Hosted on Hugging Face, versioned, FAIR-compliant with rich metadata; covers many
		well-known remote sensing datasets unified under one metadataset, though documentation
		depth varies slightly across tasks.
documentation	5	Paper provides all required information
metrics	5	Accuracy of classification is an appropriate metric
reference solution	4	Baselines like CLIP, BLIP, ALBEF evaluated in the paper; no constraints specified
software	0	No scripts or environment information provided
specification	4	Tasks (image classification across 27 satellite datasets) are clearly defined with multi-task
		and zero-shot framing; input/output structure is mostly standard but some task-specific
		nuances require interpretation.



# 3.8 Quantum Computing Benchmarks (QML)

A suite of benchmarks evaluating quantum hardware and algorithms on tasks such as state preparation, circuit optimization, and error correction across multiple platforms.

date: 2022-02-22

version:

 last\_updated:
 2022-02-22

 expired:
 false

 valid:
 yes

 valid date:
 2022-02-22

 ${\bf url:} \hspace{1.5cm} {\rm https://github.com/XanaduAI/qml-benchmarks}$ 

 $\begin{array}{lll} \textbf{doi:} & 10.48550/\mathrm{arXiv.2307.03901} \\ \textbf{domain:} & \mathrm{Quantum\ Computing} \\ \end{array}$ 

focus: Quantum algorithm performance evaluation

keywords: - quantum circuits - state preparation - error correction

licensing: Apache-2.0

task\_types:
- Circuit benchmarking - State classification
ai capability measured:
- Quantum algorithm performance and fidelity

metrics:- Fidelity - Success probabilitymodels:- IBM Q - IonQ - AQT@LBNLml\_motif:- Performance Evaluation

type: Benchmark

ml\_task: - Supervised Learning solutions: Varies per benchmark

notes: Hardware-agnostic, application-level metrics. The citation may not be correct.

contact.name: Xanadu AI

contact.email: support@xanadu.ai

datasets.links.name: PennyLane QML Benchmarks Datasets

datasets.links.url: https://pennylane.ai/datasets/collection/qml-benchmarks results.links.name: QML Benchmarks GitHub Repository (Results section)

results.links.url: https://github.com/XanaduAI/qml-benchmarks#results-and-leaderboards

fair.reproducible: True fair.benchmark ready: True

id: quantum\_computing\_benchmarks\_qml

Citations: [8]

#### Ratings:

Rating	Value	Reason
dataset	4	Datasets are accessible, but not split.
documentation	1	Only the task is defined.
metrics	3	Partially defined, somewhat inferrable metrics. Unknown whether a system's performance
		is captured.
reference_solution	0	Not provided
software	4	Run instructions exist, but are not easy to follow
specification	3	No system constraints. Task clarity and dataset format are not clearly specified.

Quantum Computing Benchmarks (QML)



# 3.9 OCP (Open Catalyst Project)

The Open Catalyst Project (OC20 and OC22) provides DFT-calculated catalyst-adsorbate relaxation datasets, challenging ML models to predict energies and forces for renewable energy applications.

date: 2020-10-20

version:

 last\_updated:
 2020-10-20

 expired:
 false

 valid:
 yes

 valid date:
 2020-10-20

url: https://opencatalystproject.org/

doi: unknown

domain: Chemistry; Materials Science

focus: Catalyst adsorption energy prediction

**keywords:** - DFT relaxations - adsorption energy - graph neural networks

licensing: OCP Terms of Use

task\_types:- Energy prediction - Force predictionai capability measured:- Prediction of adsorption energies and forces

metrics: - MAE (energy) - MAE (force)

models: - CGCNN - SchNet - DimeNet++ - GemNet-OC

ml\_motif: - Chemistry type: Benchmark

ml task: - Supervised Learning

solutions: 0

notes: Public leaderboards; active community development

contact.name:unknowncontact.email:unknowndatasets.links.name:OCP Dataset

datasets.links.url: https://fair-chem.github.io/catalysts/datasets/summary

results.links.name: OCP Pretrained Models

results.links.url: https://fair-chem.github.io/catalysts/models.html

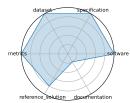
fair.reproducible: True fair.benchmark ready: True

id: ocp\_open\_catalyst\_project

Citations: [9], [10], [11], [12]

Rating	Value	Reason
dataset	5	Fully FAIR- OC20, per-adsorbate trajectories, and OC22 are versioned; datasets come
		with standardized splits, metadata, and are downloadable.
documentation	1	Paper exists, but content is behind a paywall.
metrics	5	MAE (energy and force) are standard and reproducible.
reference solution	4	Multiple baselines (GemNet-OC, DimeNet++, etc.) implemented and evaluated. No
_		hardware listed.
software	5	Data provided in Github links
specification	5	Tasks (energy and force prediction) are clearly defined with explicit I/O specifications,
		constraints, and physical relevance for renewable energy.





# $3.10 \quad MedQA$

MedQA is a large-scale multiple-choice dataset drawn from professional medical board exams (e.g., USMLE), testing AI systems on diagnostic and medical knowledge questions in English and Chinese.

date: 2020-09-28

version:

 last\_updated:
 2020-09-28

 expired:
 false

 valid:
 yes

 valid date:
 2020-09-28

 url:
 https://arxiv.org/abs/2009.13081

 doi:
 10.48550/arXiv.2009.13081

 domain:
 Medical Question Answering

 focus:
 Medical board exam QA

keywords:
- USMLE - diagnostic QA - medical knowledge - multilingual licensing:
Under Association for the Advancement of Artificial Intelligence

task types: - Multiple choice

ai capability measured: - Medical diagnosis and knowledge retrieval

metrics: - Accuracy

models: - Neural reader - Retrieval-based QA systems

ml motif: - Medical diagnosis

type: Benchmark

ml\_task: - Supervised Learning

solutions: 0

notes: Multilingual (English, Simplified and Traditional Chinese)

contact.name: Di Jin

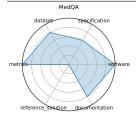
contact.email: jindi15@mit.edu

datasets.links.name: Github

datasets.links.url: https://github.com/jind11/MedQA

results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark\_ready: True
id: medqa
Citations: [13]

Rating	Value	Reason
dataset	4	Dataset is publicly available (GitHub, paper, Hugging Face), well-structured. However, versioning and metadata could be more standardized to fully meet FAIR criteria.
documentation	4	Paper is available. Evaluation criteria are not mentioned.
metrics	5	Uses clear, quantitative metric (accuracy), standard for multiple-choice benchmarks; easily comparable across models.
reference solution	0	No reference solution mentioned.
software	5	All code available on the github
specification	3	Task is clearly defined as multiple-choice QA for medical board exams; input and output formats are explicit; task scope is rigorous and structured. System constraints not specified.



# 3.11 Materials Project

The Materials Project provides an open-access database of computed properties for inorganic materials via high-throughput density functional theory (DFT), accelerating materials discovery.

date: 2011-10-01

version:

 last\_updated:
 2011-10-01

 expired:
 false

 valid:
 yes

 valid date:
 2011-10-01

url: https://materialsproject.org/

doi:unknowndomain:Materials Science

focus: DFT-based property prediction

keywords:
- DFT - materials genome - high-throughput
licensing:
https://next-gen.materialsproject.org/about/terms

task types: - Property prediction

ai capability measured: - Prediction of inorganic material properties

metrics: - MAE - R^2

models: - Automatminer - Crystal Graph Neural Networks

ml motif: - Material properties

type: Benchmark

ml task: - Supervised Learning

solutions: 0

notes: Core component of the Materials Genome Initiative

contact.name: unknown contact.email: unknown

datasets.links.name: Materials Project Catalysis Explorer

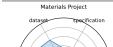
datasets.links.url: https://next-gen.materialsproject.org/catalysis

results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark ready: True

id: \_\_\_\_ materials\_project

Citations: [14]

Rating	Value	Reason
dataset	3	API key required to access data. No predefined splits.
documentation	0	No explanations or paper provided
metrics	5	Uses numerical metrics like MAE and $R^2$
reference_solution	2	Numerous models (e.g., Automatminer, CGCNN) trained on the database, but no con-
		straints or documentation listed.
software	0	No instructions available
specification	1.5	The platform offers a wide range of material property prediction tasks, but task framing and I/O formats vary by API use and are not always standardized across use cases.



eference solution documentation

# 3.12 GPQA Diamond

GPQA is a dataset of 448 challenging, multiple-choice questions in biology, physics, and chemistry, written by domain experts. It is Google-proof - experts score 65% (74% after error correction) while skilled non-experts with web access score only 34%. State-of-the-art LLMs like GPT-4 reach around 39% accuracy.

date: 2023-11-20

version:

 last\_updated:
 2023-11-20

 expired:
 false

 valid:
 yes

 valid\_date:
 2023-11-20

url: https://arxiv.org/abs/2311.12022 doi: 10.48550/arXiv.2311.12022

domain: Science

focus: Graduate-level scientific reasoning

keywords: - Google-proof - graduate-level - science QA - chemistry - physics

licensing: unknown

task\_types:
- Multiple choice - Multi-step QA
- Scientific reasoning, deep knowledge

metrics: - Accuracy

models:
- o1 - DeepSeek-R1
ml motif:
- Science and STEM fields

type: Benchmark

ml task: - Supervised Learning

 ${f solutions:} 0$   ${f notes:} Good$ 

contact.name: Julian Michael contact.email: julianjm@nyu.edu

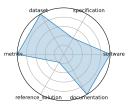
datasets.links.name:unknowndatasets.links.url:unknownresults.links.name:unknownresults.links.url:unknownfair.reproducible:Truefair.benchmarkready:

id: gpqa\_diamond

Citations: [15]

Rating	Value	Reason
dataset	5	Easily able to access dataset. Comes with predefined splits as mentioned in the paper
documentation	5	All information is listed in the associated paper
metrics	5	Each question has a correct answer, representing the tested model's performance.
reference_solution	1	Common models such as GPT-3.5 were compared. They are not open and don't provide
		requirements
software	5	Python version and requirements specified on Github site
specification	2	No system constraints or $I/O$ specified





# 3.13 ARC-Challenge (Advanced Reasoning Challenge)

The AI2 Reasoning Challenge (ARC) Challenge set comprises 7,787 natural, grade-school science questions that retrieval-based and word co-occurrence algorithms both fail, requiring advanced reasoning over a 14-million-sentence corpus.

date: 2018-03-14

version:

 last\_updated:
 2018-03-14

 expired:
 false

 valid:
 yes

 valid\_date:
 2018-03-14

url: https://allenai.org/data/arc

doi: NA domain: Science

focus: Grade-school science with reasoning emphasis

keywords: - grade-school - science QA - challenge set - reasoning

licensing: Apache 2.0 License task types: - Multiple choice

ai capability measured: - Commonsense and scientific reasoning

metrics: - Accuracy
models: - GPT-4 - Claude
ml\_motif: - Elementary science

type: Benchmark

ml task: - Supervised Learning

solutions:0notes:Goodcontact.name:unknowncontact.email:unknowndatasets.links.name:Hugging Face

datasets.links.url: https://huggingface.co/datasets/allenai/ai2\_arc

results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark ready: True

id: arc-challenge\_advanced\_reasoning\_challenge

Citations: [16]

#### Ratings:

Rating	Value	Reason
dataset	4	Data accessible, offers instructions on how to download the data via CLI tools. No splits.
documentation	5	Explains all necessary information inside a paper
metrics	5	(by default) All questions in the dataset are multiple choice, all have a correct answer
reference_solution	1	There are over 300 models listed, but very few, if any, show performance on the dataset
		or list constraints
software	0	No link to code or documentation
specification	2	Task is clear, but no constraints or format is mentioned

ARC-Challenge (Advanced Reasoning Challenge)



# 3.14 Humanity's Last Exam

Humanity's Last Exam is a multi-domain, multiple-choice benchmark containing 2,000 questions across diverse academic disciplines, designed to evaluate LLMs' ability to reason across domains without external resources.

date: 2025-01-24

version:

 last\_updated:
 2025-01-24

 expired:
 false

 valid:
 yes

 valid date:
 2025-01-24

url: https://arxiv.org/abs/2501.14249 doi: 10.48550/arXiv.2501.14249

domain: Multidomain

focus: Broad cross-domain academic reasoning

keywords: - cross-domain - academic exam - multiple-choice - multidisciplinary

licensing: MIT License
task types: - Multiple choice

ai capability measured: - Cross-domain academic reasoning

metrics:- Accuracymodels:- unkownml\_motif:- Multi-domaintype:Benchmark

ml task: - Supervised Learning

solutions: 0
notes: Good
contact.name: HLE team

contact.email: agibenchmark@safe.ai

datasets.links.name: Hugging Face

datasets.links.url: https://huggingface.co/datasets/cais/hle

results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark ready: True

id: humanitys\_last\_exam

Citations: [17]

Rating	Value	Reason
dataset	2	Data accessible through Hugging Face, but requires giving contact information to access
documentation	5	Paper available with necessary information
metrics	5	(by default) All questions in the dataset are multiple choice, all have a correct answer
${\tt reference\_solution}$	2	Performance for cutting-edge models listed, but does not specify exact version of the models or how to reproduce the result
software	4	Code for testing models posted on the github. Unknown how to run a custom model.
specification	2	Format of inputs (natural language) and outputs (multiple choice or natural language) specified. No HW constraints specified



# 3.15 FrontierMath

FrontierMath is a benchmark of hundreds of expert-vetted mathematics problems spanning number theory, real analysis, algebraic geometry, and category theory, measuring LLMs ability to solve problems requiring deep abstract reasoning.

date: 2024-11-07

version:

 last\_updated:
 2024-11-07

 expired:
 false

 valid:
 yes

 valid date:
 2024-11-07

url: https://arxiv.org/abs/2411.04872 doi: 10.48550/arXiv.2411.04872

domain: Mathematics

focus: Challenging advanced mathematical reasoning

keywords: - symbolic reasoning - number theory - algebraic geometry - category theory

licensing: unknown

task types: - Problem solving

ai capability measured: - Symbolic and abstract mathematical reasoning

metrics: - Accuracy models: - unkown

ml motif: - Math problem solving

type: Benchmark

ml task: - Supervised Learning

solutions: 0
notes: Good

contact.name: FrontierMath team contact.email: math evals@epochai.org

datasets.links.name:unknowndatasets.links.url:unknownresults.links.name:unknownresults.links.url:unknownfair.reproducible:Truefair.benchmarkready:

id: \_\_\_\_\_ frontiermath

Citations: [18]

Rating	Value	Reason
dataset	0	Paper and website had no link to any dataset. It may still exist somewhere
documentation	0	No specified way to reproduce the reference solution
metrics	5	(by default) All questions in the dataset have a correct answer
${\bf reference\_solution}$	2	Displays result of leading models on the benchmark, but none are trainable or list constraints
software	0	No link to code provided
specification	3	Well-specified process for asking questions and receiving answers. No software or hardware constraints





# 3.16 SciCode

SciCode is a scientist-curated coding benchmark with 338 subproblems derived from 80 real research tasks across 16 scientific subfields, evaluating models on knowledge recall, reasoning, and code synthesis for scientific computing tasks.

date: 2024-07-18

version:

 last\_updated:
 2024-07-18

 expired:
 false

 valid:
 yes

 valid date:
 2024-07-18

 url:
 https://arxiv.org/abs/2407.13168

 doi:
 10.48550/arXiv.2407.13168

 domain:
 Scientific Programming

focus: Scientific code generation and problem solving

keywords: - code synthesis - scientific computing - programming benchmark

licensing:unknowntask\_types:- Coding

ai capability measured: - Program synthesis, scientific computing

metrics:
- Solve rate (%)
models:
- Claude3.5-Sonnet

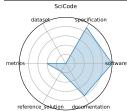
ml\_motif: - Coding type: Benchmark

ml task: - Supervised Learning

solutions:unknownnotes:Goodcontact.name:Minyang Tiancontact.email:mtian8@illinois.edudatasets.links.name:unknown

datasets.links.url: unknown
results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark\_ready: True
id: scicode
Citations: [19]

Rating	Value	Reason
dataset	0	Paper and website had no link to any dataset. It may still exist somewhere
documentation	4	Paper containing all needed info except for evaluation criteria
metrics	2	Metrics stated, but method of grading is not specified
reference_solution	1	Models presented with scores, but none are open or list constraints
software	5	Code to run exists on github repo
specification	4.5	Expected outputs and broad types of inputs stated. Few details on output grading. No HW constraints.



# 3.17 AIME (American Invitational Mathematics Examination)

The AIME is a 15-question, 3-hour exam for high-school students featuring challenging short-answer math problems in algebra, number theory, geometry, and combinatorics, assessing depth of problem-solving ability.

date: 2025-03-13

version:

 last\_updated:
 2025-03-13

 expired:
 false

 valid:
 yes

 valid date:
 2025-03-13

 ${\bf url:} \hspace*{1.5cm} {\bf https://artofproblemsolving.com/wiki/index.php/AIME\_Problems\_and\_Solutions} \\$ 

doi: NA

domain: Mathematics

focus: Pre-college advanced problem solving

**keywords:** - algebra - combinatorics - number theory - geometry

licensing: unknown

task types: - Problem solving

ai capability measured: - Mathematical problem-solving and reasoning

metrics: - Accuracy models: - unkown

ml motif: - Math problem solving

type: Benchmark

ml task: - Supervised Learning

solutions: 0

notes: Designed for human test-takers

contact.name: unknown
contact.email: unknown
datasets.links.name: AoPS website

datasets.links.url: https://artofproblemsolving.com/wiki/index.php/AIME\_Problems\_and\_Solutions

results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark ready: True

id: aime\_american\_invitational\_mathematics\_examination

Citations: [20]

Rating	Value	Reason
dataset	4	Easily accessible data with problems and solutions, but no splits
documentation	0	Not given
metrics	5	(by default) Answer is correct or it's not
reference_solution	0	Not given. Human performance stats exist, but no mentions of AI performance
software	0	No code available
specification	0	Obvious what the problems are, but not specified how to administer them to AI models.
		No HW constraints



# 3.18 MATH-500

MATH-500 is a curated subset of 500 problems from the OpenAI MATH dataset, spanning high-school to advanced levels, designed to evaluate LLMs mathematical reasoning and generalization.

date: 2025-02-15

version:

 last\_updated:
 2025-02-15

 expired:
 false

 valid:
 yes

 valid date:
 2025-02-15

url: https://huggingface.co/datasets/HuggingFaceH4/MATH-500

doi:unknowndomain:Mathematics

focus: Math reasoning generalization

keywords: - calculus - algebra - number theory - geometry

licensing: MIT License task types: - Problem solving

ai capability measured: - Math reasoning and generalization

metrics: - Accuracy
models: - unkown

ml motif: - Math problem solving

type: Benchmark

ml task: - Supervised Learning

solutions: 0

notes: Dataset hosted on Hugging Face. Data comes from a subset of OpenAI's dataset

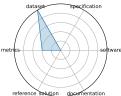
contact.name:unknowncontact.email:unknowndatasets.links.name:Hugging Face

datasets.links.url: https://huggingface.co/datasets/HuggingFaceH4/MATH-500

results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark\_ready: True
id: mathCitations: [21]

Rating	Value	Reason
dataset	5	Problems and solutions are easily downloaded. Could not find a way to download the
		data
documentation	0	Not given. Implicit instructions to download dataset.
metrics	2	Problem spec states that all of the AI reasoning steps are subject to grading, but no
		specified way to evaluate the steps
reference solution	0	Not given
software	0	No code provided
specification	0	No method of presentation and evaluation is not stated. No constraints





# 3.19 CURIE (Scientific Long-Context Understanding, Reasoning and Information Extraction)

CURIE is a benchmark of 580 problems across six scientific disciplines-materials science, quantum computing, biology, chemistry, climate science, and astrophysics- designed to evaluate LLMs on long-context understanding, reasoning, and information extraction in realistic scientific workflows.

date: 2024-04-02

version:

 last\_updated:
 2024-04-02

 expired:
 false

 valid:
 yes

 valid date:
 2024-04-02

url: https://arxiv.org/abs/2503.13517 doi: 10.48550/arXiv.2503.13517

domain: Multidomain Science

focus: Long-context scientific reasoning

keywords: - long-context - information extraction - multimodal

licensing: Apache 2.0 License

task types: - Information extraction - Reasoning - Concept tracking - Aggregation - Algebraic manipulation

- Multimodal comprehension

ai capability measured:

- Long-context understanding and scientific reasoning

metrics: - Accuracy
models: - unkown

ml motif: - Scientific problem solving

type: Benchmark

ml\_task: - Supervised Learning

 $\begin{array}{ll} \textbf{solutions:} & 0 \\ \textbf{notes:} & \textbf{Good} \end{array}$ 

contact.name: Subhashini Venugopalan contact.email: vsubhashini@google.com

datasets.links.name: unknown datasets.links.url: unknown results.links.name: unknown results.links.url: unknown fair.reproducible: True fair.benchmark ready: True

id: curie\_scientific\_long-context\_understanding\_reasoning\_and\_information\_extraction

Citations: [22]

#### Ratings:

Rating	Value	Reason
dataset	4	Dataset is available via Github, but hard to find
documentation	5	Associated paper explains all criteria
metrics	5	Quantitiative metrics such as ROUGE-L and F1 used. Metrics are tailored to the specific
		problem.
reference solution	1	Exists, but is not open
software	4	Code is available, but not well documented
specification	1	Explains types of problems in detail, but does not state exactly how to administer them.

CURIE (Scientific Long-Context Understanding, Reasoning and Information Extraction)



# 3.20 FEABench (Finite Element Analysis Benchmark)

Does not exist

date: 2023-01-26

version:

 last\_updated:
 2023-01-26

 expired:
 false

 valid:
 no

 valid date:
 2023-01-26

url: https://github.com/google/feabench

doi: unknown

domain: Computational Engineering

focus: FEA simulation accuracy and performance keywords: - finite element - simulation - PDE

licensing: unknown

 ${\bf task\_types:} \qquad \qquad {\bf -} \ {\bf Simulation} \ {\bf -} \ {\bf Performance} \ {\bf evaluation}$ 

ai\_capability\_measured: - Numerical simulation accuracy and efficiency

metrics:
- Solve time - Error norm
models:
- FEniCS - deal.II
ml\_motif:
- unknown

type: Benchmarkml task: - Supervised Learning

solutions: unknown OK notes: contact.name: unknown contact.email: unknown datasets.links.name: unknown datasets.links.url: unknown results.links.name: unknown results.links.url: unknown fair.reproducible: True fair.benchmark ready:

id: feabench\_finite\_element\_analysis\_benchmark

Citations: [23]

#### Ratings:

Rating	Value	Reason
dataset	4	Available, but not split into sets
documentation	5	In associated paper
metrics	5	Fully defined metrics
reference solution	4	Three open-source models were used. No system constraints.
software	4	Code is available, but poorly documented
specification	1.5	Output is defined and task clarity is questionable

FEABench (Finite Element Analysis Benchmark)



# 3.21 SPIQA (Scientific Paper Image Question Answering)

SPIQA assesses AI models' ability to interpret and answer questions about figures and tables in scientific papers by integrating visual and textual modalities with chain-of-thought reasoning.

date: 2024-07-12

version:

 last\_updated:
 2024-07-12

 expired:
 false

 valid:
 yes

 valid date:
 2024-07-12

url: https://arxiv.org/abs/2407.09413 doi: 10.48550/arXiv.2407.09413

domain: Computer Science

focus: Multimodal QA on scientific figures

keywords: - multimodal QA - figure understanding - table comprehension - chain-of-thought

licensing: Apache 2.0 License

task types: - Question answering - Multimodal QA - Chain-of-Thought evaluation

ai capability measured: - Visual-textual reasoning in scientific contexts

metrics: - Accuracy - F1 score

models: - Chain-of-Thought models - Multimodal QA systems

ml motif: - Scientific paper reading

type: Benchmark

ml task: - Supervised Learning

 $\mathbf{solutions}$ : 0 Good

contact.name: Subhashini Venugopalan contact.email: vsubhashini@google.com

datasets.links.name: Hugging Face

datasets.links.url: https://huggingface.co/datasets/google/spiqa

results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark ready: True

id: spiqa\_scientific\_paper\_image\_question\_answering

Citations: [24]

#### Ratings:

Rating	Value	Reason
dataset	4.5	Dataset is available (via paper/appendix), includes train/test/valid split. FAIR-compliant with minor gaps in versioning or access standardization.
documentation	5	All information provided in paper
metrics	5	Uses quantitative metrics (Accuracy, F1) aligned with the task
${\bf reference\_solution}$	2	Multiple model results (e.g., GPT-4V, Gemini) reported; baselines exist, but full runnable code not confirmed for all.
software	0	Not provided
specification	5	Task administration clearly defined; prompt instructions explicitly given, no ambiguity in format or scope.

SPIQA (Scientific Paper Image Question Answering)



# 3.22 BaisBench (Biological AI Scientist Benchmark)

BaisBench evaluates AI scientists' ability to perform data-driven biological research by annotating cell types in single-cell datasets and answering MCQs derived from biological study insights, measuring autonomous scientific discovery.

date: 2025-05-13

version:

 last\_updated:
 2025-05-13

 expired:
 false

 valid:
 yes

 valid\_date:
 2025-05-13

url:https://arxiv.org/abs/2505.08341doi:10.48550/arXiv.2505.08341domain:Computational Biologyfocus:Omics-driven AI research tasks

keywords: - single-cell annotation - biological QA - autonomous discovery

licensing: MIT License

task\_types:

ai\_capability\_measured:

metrics:

- Cell type annotation - Multiple choice
- Autonomous biological research capabilities
- Annotation accuracy - QA accuracy

models: - LLM-based AI scientist agents

ml\_motif: - Scientific research

type: Benchmark

ml\_task: - Supervised Learning

solutions: 0

notes: Underperforms human experts; aims to advance AI-driven discovery

contact.name: Xuegong Zhang

contact.email: zhangxg@mail.tsinghua.edu.cn

datasets.links.name: Github

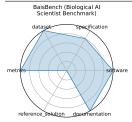
datasets.links.url: https://github.com/EperLuo/BaisBench

results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark ready: True

id: baisbench\_biological\_ai\_scientist\_benchmark

Citations: [25]

Rating	Value	Reason
dataset	5	Uses public scRNA-seq datasets linked in paper appendix; structured and accessible,
		though versioning and full metadata not formalized per FAIR standards.
documentation	5	Dataset and paper accessible; IPYNB files for setup are available on the github repo.
metrics	5	Includes precise and interpretable metrics (annotation and QA accuracy); directly aligned
		with task outputs and benchmarking goals.
reference_solution	0	Model evaluations and LLM agent results discussed; however, no fully packaged, runnable
_		baseline confirmed yet.
software	5	Instructions for environment setup available
specification	4	Task clearly defined-cell type annotation and biological QA; input/output formats are
		well-described; system constraints are not quantified.



# 3.23 MOLGEN

MolGen is a pre-trained molecular language model that generates chemically valid molecules using SELFIES and reinforcement learning, guided by chemical feedback to optimize properties such as logP, QED, and docking score.

date: 2023-01-26

version:

 last\_updated:
 2023-01-26

 expired:
 false

 valid:
 yes

 valid date:
 2023-01-26

url: https://github.com/zjunlp/MolGen

doi: 10.48550/arXiv.2301.11259 domain: Computational Chemistry

focus: Molecular generation and optimization
keywords: - SELFIES - GAN - property optimization

licensing: MIT License

task\_types:
Distribution learning - Goal-oriented generation
ai capability measured:
Generation of valid and optimized molecular structures

metrics: - Validity% - Novelty% - QED - Docking score

models: - MolGen

ml motif: - Chemical generation

type: Benchmark

ml task: - Supervised Learning

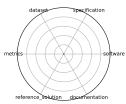
solutions: 0

notes: This is a model, not a benchmark

contact.name: unknown contact.email: unknown datasets.links.name: unknown datasets.links.url: unknown results.links.name: unknown results.links.url: unknown fair.reproducible: True fair.benchmark ready: True id: molgen Citations: [26]

Rating	Value	Reason
dataset	0	This is a pre-trained model
documentation	0	This is a pre-trained model
metrics	0	This is a pre-trained model
reference solution	0	This is a pre-trained model
software	0	This is a pre-trained model
specification	0	This is a pre-trained model





# 3.24 Open Graph Benchmark (OGB) - Biology

OGB-Biology is a suite of large-scale biological network datasets (protein-protein interaction, drug-target, etc.) with standardized splits and evaluation protocols for node, link, and graph property prediction tasks.

date: 2020-05-02

version:

 last\_updated:
 2020-05-02

 expired:
 false

 valid:
 yes

 valid date:
 2020-05-02

url: https://ogb.stanford.edu/docs/home/

doi: 10.48550/arXiv.2005.00687

domain: Graph ML

focus: Biological graph property prediction

keywords: - node prediction - link prediction - graph classification

licensing: MIT License

task types: - Node property prediction - Link property prediction - Graph property prediction

ai capability measured: - Scalability and generalization in graph ML for biology

 $\begin{array}{lll} \textbf{metrics:} & - \ Accuracy - \ ROC\text{-}AUC \\ \textbf{models:} & - \ GCN - \ GraphSAGE - \ GAT \\ \end{array}$ 

ml motif: - Chemical biology

type: Benchmark

ml task: - Supervised Learning

solutions: 0

notes: Community-driven updates

contact.name: OGB Team

 $\begin{array}{ll} \textbf{contact.email:} & \text{ogb@cs.stanford.edu} \\ \textbf{datasets.links.name:} & \text{OGB Webpage} \end{array}$ 

datasets.links.url: https://ogb.stanford.edu/docs/dataset\_overview/

results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark ready: True

id: open\_graph\_benchmark\_ogb\_-\_biology

Citations: [27]

Rating	Value	Reason
dataset	5	Fully FAIR- datasets are versioned, split, and accessible via a standardized API; extensive metadata and documentation are included.
1	-	
documentation	5	All necessary information is included in a paper.
metrics	5	Reproducible, quantitative metrics (e.g., ROC-AUC, accuracy) that are tightly aligned with the tasks.
${\tt reference\_solution}$	3	Multiple baselines implemented and documented (GCN, GAT, GraphSAGE). No contraints.
software	5	All necessary information is provided on the Github
specification	4	Tasks (node/link/graph property prediction) are clearly specified with input/output formats and standardized protocols; constraints (e.g., splits) are well-defined. No constraints.





# 3.25 JARVIS-Leaderboard

JARVIS-Leaderboard is a community-driven platform benchmarking AI, electronic structure, force-fields, quantum computing, and experimental methods across hundreds of materials science tasks.

date: 2023-06-20

version:

 last\_updated:
 2023-06-20

 expired:
 false

 valid:
 yes

 valid date:
 2023-06-20

 url:
 https://arxiv.org/abs/2306.11688

 doi:
 10.48550/arXiv.2306.11688

 domain:
 Materials Science; Benchmarking

focus: Comparative evaluation of materials design methods keywords: - leaderboards - materials methods - simulation

licensing: NIST

task types: - Method benchmarking - Leaderboard ranking

ai capability measured: - Performance comparison across diverse materials design methods

metrics: - MAE - RMSE - Accuracy

models:
- unkown
ml\_motif:
- Material science
type:
- Benchmark

ml task: - Supervised Learning

solutions: 0

notes: 1281 contributions across 274 benchmarks

contact.name: Kamal Choudhary
contact.email: kamal.choudhary@nist.gov
datasets.links.name: AI model specific benchmarks

datasets.links.url: https://pages.nist.gov/jarvis\_leaderboard/AI/

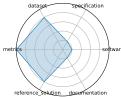
results.links.name: unknown
results.links.url: unknown
fair.reproducible: True
fair.benchmark ready: True

id: jarvis-leaderboard

Citations: [28]

Rating	Value	Reason
dataset	4	Data is public and adheres to FAIR principles across the NIST-hosted infrastructure;
		however, metadata completeness varies slightly across benchmarks. No splits.
documentation	1	Only the task is specified.
metrics	5	Metrics stated for each benchmark.
reference solution	4	Many baselines across tasks (CGCNN, ALIGNN, M3GNet, etc.); no constraints specified.
software	1	Setup script provided, but no code provided
specification	1	Only dataset format is defined.





# 3.26 Nixtla Neural Forecast TimeGPT

TimeGPT is a transformer-based generative pretrained model on 100B+ time series data for zero-shot forecasting and anomaly detection via API .

 date:
 2023-10-05

 version:
 v3.0.2

 last\_updated:
 2025-06

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2023-10-05

 ${\bf url:} \hspace{1.5cm} {\rm https://github.com/Nixtla/neuralforecast}$ 

 $\begin{array}{lll} \mbox{\bf doi:} & 10.48550/\mbox{arXiv.}2310.03589 \\ \mbox{\bf domain:} & \mbox{Time-series; General ML} \\ \end{array}$ 

focus: Time-series foundation model "TimeGPT" for forecasting and anomaly detection

**keywords:** - TimeGPT - foundation model - time-series - generative model

licensing: Apache License 2.0

task\_types:

ai\_capability\_measured:
metrics:
Time-series forecasting - Anomaly detection
Zero-shot forecasting - anomaly detection
RMSE - Anomaly detection metrics

models:
 - TimeGPT
ml\_motif:
 - Time-series
type:
 Platform
ml\_task:
 - Forecasting

solutions: Solution details are described in the referenced paper or repository.

notes: Offered via Nixtla API and Azure Studio; enterprise-grade support available.

contact.name: Azul Garza (Nixtla)

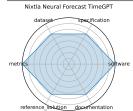
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: nixtla neural forecast timegpt

Citations: [29]

Rating	Value	Reason
dataset	3	Evaluated on existing open datasets, but consolidated data release, splits, and FAIR
		metadata are not provided.
documentation	3	Basic README with installation and usage examples; more detailed API docs and tutorials would improve usability.
metrics	4	Uses standard forecasting metrics such as RMSE, MASE, SMAPE, and anomaly detection metrics consistently across evaluations.
$reference\_solution$	3	TimeGPT implementation is available, but baseline comparisons and additional reference models are limited.
software	4	Fully open-source Apache 2.0 implementation integrated in NeuralForecast, supporting training and evaluation via API. Production-grade deployment available via Nixtla API and Azure.
specification	3	Concept and forecasting goals are described, but formal input/output definitions and task constraints are not rigorously specified.



# 3.27 Nixtla Neural Forecast NHITS

NHITS (Neural Hierarchical Interpolation for Time Series) is a state-of-the-art model that improved accuracy by  $^225\%$  and reduced compute by 50x compared to Transformer baselines, using hierarchical interpolation and multi-rate sampling .

 date:
 2023-06-01

 version:
 v3.0.2

 last\_updated:
 2025-06

 expired:
 unknown

 valid:
 yes

 valid date:
 2023-06-01

 ${\bf url:} \hspace{1.5cm} {\rm https://github.com/Nixtla/neuralforecast}$ 

doi: unknown

domain: Time-series; General ML

focus: Official NHITS implementation for long-horizon time series forecasting keywords:

- NHITS - long-horizon forecasting - neural interpolation - time-series

licensing: Apache License 2.0 task types: - Time-series forecasting

ai capability measured: - Accuracy - compute efficiency for long series

metrics: - RMSE - MAPE

models:- NHITSml\_motif:- Time-seriestype:Platformml\_task:- Forecasting

solutions: 0

notes: Official implementation in NeuralForecast, included since its AAAI 2023 release.

contact.name: Kin G. Olivares (Nixtla)

contact.email: unknown

datasets.links.name: Standard forecast datasets, M4

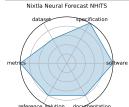
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: nixtla\_neural\_forecast\_nhits

Citations: [30]

Rating	Value	Reason
dataset	3	Uses standard benchmark datasets like M4, but does not bundle them directly. FAIR
		compliance depends on external dataset sources and user setup.
documentation	4	Well-documented on GitHub and in AAAI paper, with code examples, training guidance,
		and usage tutorials. More model-specific docs could improve clarity further.
metrics	5	Evaluated using RMSE, MAPE, and other standard forecasting metrics, integrated into
		training and evaluation APIs.
reference_solution	4	Official NHITS implementation is fully reproducible with training/eval configs, though
		pretrained weights are not always provided.
software	5	Implemented within the open-source NeuralForecast library under Apache 2.0. Includes
		training, evaluation, and hyperparameter tuning pipelines. Actively maintained.
specification	5	The NHITS forecasting task is clearly defined with structured input/output formats.
		Model design targets long-horizon accuracy and compute efficiency.



# 3.28 Nixtla Neural Forecast TimeLLM

Time-LLM uses reprogramming layers to adapt frozen LLMs for time series forecasting, treating forecasting as a language task

.

 date:
 2023-10-03

 version:
 v3.0.2

 last\_updated:
 2025-06

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2023-10-03

 ${\bf url:} \hspace{1.5cm} {\rm https://github.com/Nixtla/neuralforecast}$ 

 $\begin{array}{lll} \mbox{\bf doi:} & 10.48550/\mbox{arXiv.}2310.01728 \\ \mbox{\bf domain:} & \mbox{Time-series; General ML} \\ \end{array}$ 

focus: Reprogramming LLMs for time series forecasting

keywords: - Time-LLM - language model - time-series - reprogramming

licensing: Apache License 2.0
task\_types: - Time-series forecasting

ai capability measured: - Model reuse via LLM - few-shot forecasting

metrics:- RMSE - MAPEmodels:- Time-LLMml\_motif:- Time-seriestype:Platformml\_task:- Forecasting

solutions: Solution details are described in the referenced paper or repository.

notes: Fully open-source; transforms forecasting using LLM text reconstruction.

contact.name: Ming Jin (Nixtla)

contact.email: unknown

datasets.links.name: Standard forecast datasets, M4

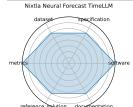
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: nixtla\_neural\_forecast\_timellm

Citations: [31]

Rating	Value	Reason
dataset	3	Evaluated on standard datasets like M4 and ETT, but dataset splits and versioning are
		not bundled or explicitly FAIR-compliant.
documentation	3	GitHub README provides installation and quick usage examples, but lacks detailed API
		docs, training walkthroughs, or extended tutorials.
metrics	4	Standard forecasting metrics such as RMSE, MAPE, and SMAPE are reported. Evalua-
		tion is consistent, though deeper metric justification is limited.
reference_solution	3	Time-LLM implementation is open and reproducible, but limited baselines or comparative
		implementations are included directly.
software	4	Fully open-source under Apache 2.0, integrated into the NeuralForecast library. Includes
		Time-LLM implementation with example usage and training scripts.
specification	3	High-level framing of forecasting as language modeling is clear, but detailed input/output
		specifications, constraints, and task formalization are minimal.



# 3.29 Nixtla NeuralForecast

NeuralForecast offers scalable, user-friendly implementations of over 30 neural forecasting models (NBEATS, NHITS, TFT, DeepAR, etc.), emphasizing quality, usability, interpretability, and performance.

 date:
 2022-04-01

 version:
 v3.0.2

 last\_updated:
 2025-06

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2022-04-01

 ${\bf url:} \hspace{1.5cm} {\rm https://github.com/Nixtla/neuralforecast}$ 

doi: unknown

domain: Time-series forecasting; General ML

focus: High-performance neural forecasting library with >30 models

keywords: - time-series - neural forecasting - NBEATS, NHITS, TFT - probabilistic forecasting - usability

licensing: Apache License 2.0 task types: - Time-series forecasting

ai capability measured: - Forecast accuracy - interpretability - speed

metrics: - RMSE - MAPE - CRPS

models: - NBEATS - NHITS - TFT - DeepAR

ml\_motif: - Time-series
type: Platform
ml\_task: - Forecasting

solutions: 0

notes: AutoModel supports hyperparameter tuning and distributed execution via Ray and Optuna.

First official NHITS implementation. contentReference oaicite:4 ndex=4

contact.name: Kin G. Olivares (Nixtla)

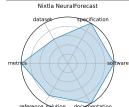
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: nixtla neuralforecast

Citations: [32]

Rating	Value	Reason
dataset	3	NeuralForecast does not include its own datasets but supports standard datasets (e.g.,
		M4, M5, ETT). FAIR compliance depends on user-supplied data.
documentation	5	Rich documentation with examples, API references, tutorials, notebooks, and CLI sup-
		port. PyPI, GitHub, and official blog posts offer clear guidance for usage and extension.
metrics	5	RMSE, MAPE, CRPS, and other domain-relevant metrics are well supported and inte-
		grated into the evaluation loop.
reference_solution	4	Includes runnable model baselines and training scripts for all supported models. Some
		models have pretrained weights, but not all are fully benchmarked out-of-the-box.
software	5	Actively maintained open-source library under Apache 2.0. Offers a clean API, extensive
		model zoo (>30 models), integration with Ray, Optuna, and supports scalable training
		and inference workflows.
specification	5	Forecasting task is well-defined with clear input/output structures. Framework supports
		probabilistic and deterministic forecasting, with unified interfaces and support for batch
		evaluation.



# 3.30 vLLM Performance Dashboard

A live visual dashboard for vLLM showcasing throughput, latency, and other inference metrics across models and hardware configurations.

 date:
 2022-06-22

 version:
 v1.0

 last\_updated:
 2025-01

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2022-06-22

 ${\bf url:} \hspace{1.5cm} {\rm https://simon-mo-workspace.observablehq.cloud/vllm-dashboard-v0/llm-$ 

doi: unknown

domain: LLM; HPC/inference

focus: Interactive dashboard showing inference performance of vLLM

keywords: - Dashboard - Throughput visualization - Latency analysis - Metric tracking

licensing: unknown

task types: - Performance visualization

ml\_motif: - HPC/inference
type: Framework
ml\_task: - Visualization

solutions: 0

notes: Built using ObservableHQ; integrates live data from vLLM benchmarks. The URL requires a

login to access the content.

contact.name: Simon Mo
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: vllm\_performance\_dashboard

Citations: [33]

Rating	Value	Reason
dataset	2	No datasets are bundled; the dashboard visualizes metrics derived from model inference
		logs or external endpoints, not a formal dataset.
documentation	4	Public dashboard with instructions and tooltips; documentation is clear, though access is
		restricted (login required) and backend setup is opaque to users.
metrics	4	Tracks tokens/sec, TTFT, memory usage, and platform comparisons. Metrics are clear
		but focused on visualization rather than statistical robustness.
reference_solution	3	Dashboards include reproducible views of benchmarked models, but do not ship with
		runnable model code. Relies on external serving infrastructure.
software	4	Interactive dashboard built with ObservableHQ and linked to vLLM benchmarks. Source
		code is not fully open, but backend integration with vLLM is well-maintained.
specification	4	While primarily a visualization tool, it includes benchmark configurations, metric defini-
		tions, and supports comparison across models and hardware.



# 3.31 vLLM Inference and Serving Engine

vLLM is a fast, high-throughput, memory-efficient inference and serving engine for large language models, featuring PagedAttention, continuous batching, and support for quantized and pipelined model execution. Benchmarks compare it to TensorRT-LLM, SGLang, and others.

 date:
 2023-09-12

 version:
 v0.10.0

 last\_updated:
 2025-06

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2023-09-12

url: https://github.com/vllm-project/vllm/tree/main/benchmarks

doi: unknown

domain: LLM; HPC/inference

focus: High-throughput, memory-efficient inference and serving engine for LLMs keywords: - LLM inference - PagedAttention - CUDA graph - streaming API - quantization

licensing: Apache License 2.0 task types: - Inference Benchmarking

ai\_capability\_measured: - Throughput - latency - memory efficiency

metrics: - Tokens/sec - Time to First Token (TTFT) - Memory footprint

models: - LLaMA - Mixtral - FlashAttention-based models

 ml\_motif:
 - HPC/inference

 type:
 Framework

 ml\_task:
 - Inference

 solutions:
 0

notes: Incubated by LF AI and Data; achieves up to 24x throughput over HuggingFace Transformers

contact.name: Woosuk Kwon (vLLM Team)

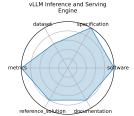
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: vllm\_inference\_and\_serving\_engine

Citations: [34]

Rating	Value	Reason
dataset	3	No traditional dataset is included. Instead, it uses structured configs and logs suitable
		for inference benchmarking. FAIR principles are only partially applicable.
documentation	4	Well-structured GitHub documentation with setup instructions, config examples, bench-
		marking comparisons, and performance tuning guides.
metrics	5	Comprehensive performance metrics like tokens/sec, time-to-first-token (TTFT), and
		memory footprint are consistently applied and benchmarked across frameworks.
$reference\_solution$	4	Provides runnable scripts and configs for several models (LLaMA, Mixtral, etc.) across
_		platforms. Baselines are reproducible, though not all models are fully wrapped or hosted.
software	5	Actively maintained open-source project under Apache 2.0. GitHub repo includes full
		serving engine, benchmarking scripts, CUDA integration, and deployment examples.
specification	5	Inference benchmarks are well-defined with clear input/output formats and platform-
		specific constraints. Covers multiple models, hardware backends, and batching configu-
		rations.



# 3.32 SGLang Framework

A high-performance open-source serving framework combining efficient backend runtime (RadixAttention, batching, quantization) and expressive frontend language, boosting LLM/VLM inference throughput up to  $\tilde{\ }$ 3x over alternatives.

 date:
 2023-12-12

 version:
 v0.4.9

 last\_updated:
 2025-06

 expired:
 unknown

 valid:
 yes

 valid date:
 2023-12-12

 ${\bf url:} \\ {\bf https://github.com/sgl-project/sglang/tree/main/benchmark}$ 

doi: 10.48550/arXiv.2312.07104

domain: LLM Vision

focus: Fast serving framework for LLMs and vision-language models

keywords: - LLM serving - vision-language - RadixAttention - performance - JSON decoding

licensing:Apache License 2.0task types:- Model serving framework

ai capability measured: - Serving throughput - JSON/task-specific latency

metrics: - Tokens/sec - Time-to-first-token - Throughput gain vs baseline

models: - LLaVA - DeepSeek - Llama

ml\_motif: - LLM Vision
type: Framework
ml task: - Model serving

solutions: Solution details are described in the referenced paper or repository.

notes: Deployed in production (xAI, NVIDIA, Google Cloud); v0.4.8 release June 2025.

contact.name: SGLang Team unknown

datasets.links.name: Benchmark configs results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: sglang\_framework

Citations: [35]

Rating	Value	Reason
dataset	2	Does not introduce new datasets; instead, it evaluates performance using existing model
		benchmarks. Only configuration files are included.
documentation	4	Strong GitHub documentation, install guides, and benchmarks. Some advanced topics
		(e.g., scaling, hardware tuning) could use deeper walkthroughs.
metrics	5	Serving-related metrics such as tokens/sec, time-to-first-token, and throughput gain vs.
		baselines are well-defined and consistently applied.
reference solution	3	Provides benchmark configs and example integrations (e.g., with LLaVA, DeepSeek), but
_		not all models or scripts are runnable out-of-the-box.
software	5	Actively maintained and production-deployed (e.g., xAI, NVIDIA); source code available
		under Apache 2.0. Includes efficient backends (RadixAttention, quantization, batching)
		and full serving infrastructure.
specification	4	The framework clearly defines performance targets, serving logic, and model integration.
		Input/output expectations are consistent, but not all benchmarks are standardized.



# 3.33 Jet Classification

This benchmark evaluates ML models for real-time classification of particle jets using high-level features derived from simulated LHC data. It includes both full-precision and quantized models optimized for FPGA deployment.

 date:
 2024-05-01

 version:
 v0.2.0

 last\_updated:
 2024-05

 expired:
 unknown

 valid:
 yes

 valid date:
 2024-05-01

 ${\bf url:} \qquad \qquad {\rm https://github.com/fastmachinelearning/fastml-science/tree/main/jet-classify}$ 

doi: 10.48550/arXiv.2207.07958

domain: Particle Physics

focus: Real-time classification of particle jets using HL-LHC simulation features

keywords: - classification - real-time ML - jet tagging - QKeras

licensing: Apache License 2.0 task\_types: - Classification

ai capability measured: - Real-time inference - model compression performance

metrics: - Accuracy - AUC

models: - Keras DNN - QKeras quantized DNN

 $ml\_motif:$  - Real-time type: Benchmark

ml task: - Supervised Learning

solutions: Solution details are described in the referenced paper or repository.

notes: Includes both float and quantized models using QKeras

contact.name: Jules Muhizi contact.email: unknown datasets.links.name: JetClass

datasets.links.url: https://zenodo.org/record/6619768

results.links.name: ChatGPT LLM

 $\textbf{results.links.url:} \\ \text{https://docs.google.com/document/d/1runrcij-eoH3\_lgGZ8wm2z1YbL1Qf5cSNbVbHyWFDs4} \\ \text{-} \\ \text{-$ 

fair.reproducible: True fair.benchmark ready: True

id: \_\_\_\_ jet\_classification

Citations: [36]

Rating	Value	Reason
dataset	5	None
documentation	4	Full reproducibility requires manual setup
metrics	5	None
reference solution	4	HW/SW requirements missing; Reference not bundled as official starter kit
software	3	Not containerized; Setup automation/documentation could be improved
specification	4	System constraints missing



# 3.34 Irregular Sensor Data Compression

This benchmark addresses lossy compression of irregularly sampled sensor data from particle detectors using real-time autoencoder architectures, targeting latency-critical applications in physics experiments.

 date:
 2024-05-01

 version:
 v0.2.0

 last\_updated:
 2024-05

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2024-05-01

 ${\bf url:} \qquad \qquad {\rm https://github.com/fastmachinelearning/fastml-science/tree/main/sensor-data-compression}$ 

doi: 10.48550/arXiv.2207.07958

domain: Particle Physics

focus: Real-time compression of sparse sensor data with autoencoders keywords: - compression - autoencoder - sparse data - irregular sampling

licensing: Apache License 2.0 task types: - Compression

ai capability measured: - Reconstruction quality - compression efficiency

metrics: - MSE - Compression ratio

models: - Autoencoder - Quantized autoencoder

ml motif: - Real-time, Image/CV

type: Benchmark

ml task: - Unsupervised Learning

solutions: Solution details are described in the referenced paper or repository.

notes: Based on synthetic but realistic physics sensor data

contact.name: Ben Hawks, Nhan Tran

contact.email: unknown

datasets.links.name: Custom synthetic irregular sensor dataset

datasets.links.url: https://github.com/fastmachinelearning/fastml-science/tree/main/sensor-data-compression

results.links.name: ChatGPT LLM

fair.reproducible: True fair.benchmark ready: True

id: irregular\_sensor\_data\_compression

Citations: [37]

Rating	Value	Reason
dataset	5	All criteria met
documentation	4	Setup for deployment (e.g., FPGA pipeline) requires familiarity with tooling
metrics	5	All criteria met
reference_solution	4	Not fully documented or automated for reproducibility
software	3	Not containerized; Full automation and documentation could be improved
specification	4	Exact latency or resource constraints not numerically specified





# 3.35 Beam Control

Beam Control explores real-time reinforcement learning strategies for maintaining stable beam trajectories in particle accelerators. The benchmark is based on the BOOSTR environment for accelerator simulation.

 date:
 2024-05-01

 version:
 v0.2.0

 last\_updated:
 2024-05

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2024-05-01

 ${\bf url:} \qquad \qquad {\rm https://github.com/fastmachinelearning/fastml-science/tree/main/beam-control}$ 

 $\begin{array}{lll} \mbox{\bf doi:} & 10.48550/\mbox{arXiv}.2207.07958 \\ \mbox{\bf domain:} & \mbox{Accelerators and Magnets} \\ \end{array}$ 

focus: Reinforcement learning control of accelerator beam position keywords:

- RL - beam stabilization - control systems - simulation

licensing: Apache License 2.0

task types: - Control

ai capability measured: - Policy performance in simulated accelerator control

metrics:
- Stability - Control loss
models:
- DDPG - PPO (planned)

ml\_motif:
- Real-time, RL
type:
Benchmark

ml task: - Reinforcement Learning

solutions: Solution details are described in the referenced paper or repository.

notes: Environment defined, baseline RL implementation is in progress

contact.name: Ben Hawks, Nhan Tran

contact.email:unknownresults.links.name:ChatGPT LLMfair.reproducible:in progressfair.benchmark\_ready:in progressid:beam\_controlCitations:[38], [39]

Rating	Value	Reason
dataset	3	Not findable (no DOI/indexing); Not interoperable (format/schema unspecified)
documentation	3	Setup instructions and pretrained model details are missing
metrics	5	All criteria met
reference_solution	2	HW/SW requirements missing; Metrics not evaluated with reference; Baseline not train-
		able/open
software	1	Code not documented; Incomplete setup and not containerized
specification	4	Latency/resource constraints not fully quantified





# 3.36 Ultrafast jet classification at the HL-LHC

Demonstrates three ML models (MLP, Deep Sets, Interaction Networks) optimized for FPGA deployment with O(100 ns) inference using quantized models and hls4ml, targeting real-time jet tagging in the L1 trigger environment at the high-luminosity LHC. Data is available on Zenodo DOI:10.5281/zenodo.3602260.

 date:
 2024-07-08

 version:
 v1.0

 last\_updated:
 2024-07

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2024-07-08

 $\begin{array}{lll} \textbf{url:} & \text{https://arxiv.org/pdf/}2402.01876 \\ \textbf{doi:} & 10.48550/\text{arXiv.}2402.01876 \\ \end{array}$ 

domain: Particle Physics

focus: FPGA-optimized real-time jet origin classification at the HL-LHC

keywords: - jet classification - FPGA - quantization-aware training - Deep Sets - Interaction Networks

licensing: CC-BY task types: - Classification

ai\_capability\_measured:
 Real-time inference under FPGA constraints
 Accuracy - Latency - Resource utilization
 MLP - Deep Sets - Interaction Network

ml\_motif: - Real-time type: Model

ml task: - Supervised Learning

solutions: Solution details are described in the referenced paper or repository.

notes: Uses quantization-aware training; hardware synthesis evaluated via hls4ml

contact.name: Patrick Odagiu contact.email: podagiu@ethz.ch datasets.links.name: Zenodo dataset

datasets.links.url: https://zenodo.org/records/3602260

results.links.name: ChatGPT LLM

 $\textbf{results.links.url:} \\ \text{https://docs.google.com/document/d/1gDf1CIYtfmfZ9urv1jCRZMYz} \\ \text{3WwEETkugUC65OZBdw} \\ \text{The substitution of the lattice of the$ 

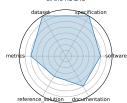
**fair.reproducible:** True **fair.benchmark ready:** False

id: ultrafast jet\_classification\_at\_the\_hl-lhc

Citations: [40]

Rating	Value	Reason
dataset	4	FAIR metadata limited; no clear mention of dataset format or splits
documentation	3	No linked GitHub repo or setup instructions; paper provides partial guidance only
metrics	3	Metrics exist (accuracy, latency, utilization), but formal definitions and evaluation guidance are limited
${\bf reference\_solution}$	2	Reference implementations not fully reproducible; no evaluation pipeline or training setup provided
software	3	Not containerized; Setup and automation incomplete
specification	4	Hardware constraints are referenced but not fully detailed or standardized





# 3.37 Quench detection

Exploration of real-time quench detection using unsupervised and RL approaches, combining multi-modal sensor data (BPM, power supply, acoustic), operating on kHz-MHz streams with anomaly detection and frequency-domain features.

 date:
 2024-10-15

 version:
 v1.0

 last\_updated:
 2024-10

 expired:
 no

 valid:
 yes

 valid date:
 2024-10-15

 $\textbf{url:} \hspace*{2.5cm} \text{https://indico.cern.ch/event/1387540/contributions/6153618/attachments/2948441/5182077/fast\_ml\_magnets\_ml_magn$ 

doi: NA

domain: Accelerators and Magnets

focus: Real-time detection of superconducting magnet quenches using ML keywords: - quench detection - autoencoder - anomaly detection - real-time

licensing: Via Fermilab

task types: - Anomaly detection - Quench localization

ai capability measured: - Real-time anomaly detection with multi-modal sensors

metrics: - ROC-AUC - Detection latency

models: - Autoencoder - RL agents (in development)

ml\_motif:
- Real-time, RL
type:
Benchmark

ml task: - Reinforcement, Unsupervised Learning

solutions: 0

notes: Precursor detection in progress; multi-modal and dynamic weighting methods

contact.name: Maira Khan contact.email: unknown

datasets.links.name: BPM and power supply data from BNL

results.links.name: ChatGPT LLM fair.reproducible: in progress fair.benchmark ready: False

id: quench\_detection

Citations: [41]

Rating	Value	Reason
dataset	2	Dataset URL is missing; FAIR principles largely unmet
documentation	2	Only a conference slide deck is available; lacks detailed instructions or repository for reproduction
metrics	3	ROC-AUC and latency are mentioned, but metric definitions and formal evaluation setup are missing
reference solution	1	No baseline or reproducible model implementation available
software	1	Code not provided; no evidence of documentation or containerization
specification	4	Real-time detection task is clearly described, but exact constraints, inputs/outputs, and evaluation protocol are only partially specified





# 3.38 Intelligent experiments through real-time AI

Research and Development demonstrator for real-time processing of high-rate tracking data from the sPHENIX detector (RHIC) and future EIC systems. Uses GNNs with hls4ml for FPGA-based trigger generation to identify rare events (heavy flavor, DIS electrons) within 10 micros latency. Demonstrated improved accuracy and latency on Alveo/FELIX platforms.

 date:
 2025-01-08

 version:
 v1.0

 last\_updated:
 2025-01

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2025-01-08

 $\begin{array}{lll} \textbf{url:} & & \text{https://arxiv.org/pdf/2501.04845} \\ \textbf{doi:} & & 10.48550/\text{arXiv.2501.04845} \\ \end{array}$ 

domain: Instrumentation and Detectors; Nuclear Physics; Particle Physics

focus: Real-time FPGA-based triggering and detector control for sPHENIX and future EIC keywords: - FPGA - Graph Neural Network - hls4ml - real-time inference - detector control

licensing: CC BY-NC-ND 4.0

task types: - Trigger classification - Detector control - Real-time inference

ai\_capability\_measured: - Low-latency GNN inference on FPGA

metrics: - Accuracy (charm and beauty detection) - Latency (micros) - Resource utilization

(LUT/FF/BRAM/DSP)

models: - Bipartite Graph Network with Set Transformers (BGN-ST) - GarNet (edge-classifier)

ml\_motif: - Real-time type: Model

ml task: - Supervised Learning

solutions: Solution details are described in the referenced paper or repository.

notes: Achieved ~97.4% accuracy for beauty decay triggers; sub-10 micros latency on Alveo U280;

hit-based FPGA design via hls4ml and FlowGNN.

contact.name: Jakub Kvapil
contact.email: Jakub.Kvapil@lanl.gov

datasets.links.name: Internal simulated tracking data (sPHENIX and EIC DIS-electron tagger)

results.links.name: ChatGPT LLM

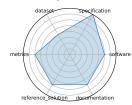
fair.reproducible: True fair.benchmark ready: False

id: intelligent\_experiments\_through\_real-time\_ai

Citations: [42]

Rating	Value	Reason
dataset	2	Dataset is internal and not publicly available or FAIR-compliant
documentation	3	No public GitHub or complete pipeline documentation
metrics	3	Metrics relevant but not supported by evaluation scripts or baselines
reference solution	3	No public or reproducible implementation released
software	3	No containerized or open-source setup provided
specification	4	Architectural/system specifications are incomplete





# 3.39 Neural Architecture Codesign for Fast Physics Applications

Introduces a two-stage neural architecture codesign (NAC) pipeline combining global and local search, quantization-aware training, and pruning to design efficient models for fast Bragg peak finding and jet classification, synthesized for FPGA deployment with hls4ml. Achieves >30x reduction in BOPs and sub-100 ns inference latency on FPGA.

 date:
 2025-01-09

 version:
 v1.0

 last\_updated:
 2025-01

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2025-01-09

url: https://arxiv.org/abs/2501.05515 doi: 10.48550/arXiv.2501.05515

domain: Physics; Materials Science; Particle Physics

focus: Automated neural architecture search and hardware-efficient model codesign for fast physics

applications

keywords: - neural architecture search - FPGA deployment - quantization - pruning - hls4ml

licensing: Via Fermilab

task types: - Classification - Peak finding

ai\_capability\_measured: - Hardware-aware model optimization; low-latency inference

metrics: - Accuracy - Latency - Resource utilization

models: - NAC-based BraggNN - NAC-optimized Deep Sets (jet)

ml motif: - Real-time, Image/CV

type: Framework

ml task: - Supervised Learning

solutions: Solution details are described in the referenced paper or repository.

notes: Demonstrated two case studies (materials science, HEP); pipeline and code open-sourced.

contact.name: Jason Weitz (UCSD), Nhan Tran (FNAL)

contact.email: unknown
results.links.name: ChatGPT LLM
fair.reproducible: Yes (nac-opt, hls4ml)

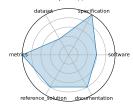
fair.benchmark ready: False

id: neural architecture codesign for fast physics applications

Citations: [43]

Rating	Value	Reason
dataset	2	Simulated datasets referenced but not publicly available or FAIR-compliant
documentation	4	Detailed paper and tools described; open repo planned but not yet complete
metrics	5	Clear, quantitative metrics aligned with task goals and hardware evaluation
${\tt reference\_solution}$	4	Models tested on hardware with source code references; full training pipeline not yet released
software	3	Toolchain (hls4ml, nac-opt) described but not yet containerized or fully packaged
specification	5	Fully specified task with constraints and target deployment; includes hardware context





# 3.40 Smart Pixels for LHC

Presents a 256x256-pixel ROIC in 28 nm CMOS with embedded 2-layer NN for cluster filtering at 25 ns, achieving 54-75% data reduction while maintaining noise and latency constraints. Prototype consumes  $^{\sim}300$  microW/pixel and operates in combinatorial digital logic.

 date:
 2024-06-24

 version:
 v1.0

 last\_updated:
 2024-06

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2024-06-24

url: https://arxiv.org/abs/2406.14860 doi: 10.48550/arXiv.2406.14860

domain: Particle Physics; Instrumentation and Detectors

focus:
On-sensor, in-pixel ML filtering for high-rate LHC pixel detectors keywords:
- smart pixel - on-sensor inference - data reduction - trigger

licensing: Via Fermilab

task types: - Image Classification - Data filtering

ai\_capability\_measured: - On-chip - low-power inference; data reduction

metrics: - Data rejection rate - Power per pixel

models:
- 2-layer pixel NN
ml motif:
- Real-time, Image/CV

type: Benchmark

ml task: - Image Classification

solutions: Solution details are described in the referenced paper or repository.

notes: Prototype in CMOS 28 nm; proof-of-concept for Phase III pixel upgrades.

contact.name: Lindsey Gray; Jennet Dickinson

contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: True

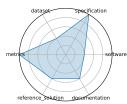
fair.benchmark\_ready: Yes (Zenodo:7331128)
id: smart\_pixels\_for\_lhc

Citations: [44]

#### Ratings:

Rating	Value	Reason
dataset	2	No dataset links; not publicly hosted or FAIR-compliant
documentation	3	Paper contains detailed descriptions, but no repo or external guide for reproducing results
metrics	5	None
${\bf reference\_solution}$	3	In-pixel 2-layer NN described and evaluated, but reproducibility and source files are not released
software	2	No packaged code or setup scripts available; replication depends on hardware description and paper
specification	5	None

Smart Pixels for LHC



## 3.41 HEDM (BraggNN)

Uses BraggNN, a deep neural network, for rapid Bragg peak localization in high-energy diffraction microscopy, achieving about 13x speedup compared to Voigt-based methods while maintaining sub-pixel accuracy.

 date:
 2023-10-03

 version:
 v1.0

 last\_updated:
 2023-10

 expired:
 unknown

 valid:
 yes

 valid date:
 2023-10-03

url: https://arxiv.org/abs/2008.08198 doi: 10.48550/arXiv.2008.08198

domain: Material Science

focus: Fast Bragg peak analysis using deep learning in diffraction microscopy

keywords: - BraggNN - diffraction - peak finding - HEDM

licensing: DOE Public Access Plan

task types: - Peak detection

ai\_capability\_measured:High-throughput peak localizationmetrics:Localization accuracy - Inference time

models: - BraggNN

ml motif: - Real-time, Image/CV

type: Frameworkml task: - Peak finding

solutions: Solution details are described in the referenced paper or repository.

notes: Enables real-time HEDM workflows; basis for NAC case study.

contact.name: Jason Weitz (UCSD)

contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: True fair.benchmark ready: True

id: hedm braggnn

Citations: [45]

Rating	Value	Reason
dataset	2	No dataset links or FAIR metadata; unclear public access
documentation	3	Paper is clear, but lacks a GitHub repo or full reproducibility pipeline
metrics	4	Only localization accuracy and inference time mentioned; not formally benchmarked with scripts
${\tt reference\_solution}$	3	BraggNN model is described and evaluated, but no direct implementation or inference scripts available
software	2	No standalone code repository or setup instructions provided
specification	5	None





## 3.42 4D-STEM

Proposes ML methods for real-time analysis of 4D scanning transmission electron microscopy datasets; framework details in progress.

 date:
 2023-12-03

 version:
 v1.0

 last\_updated:
 2023-12

 expired:
 unknown

 valid:
 yes

 valid date:
 2023-12-03

url: https://openreview.net/pdf?id=7yt3N0o0W9

doi:unknowndomain:Material Science

focus: Real-time ML for scanning transmission electron microscopy
keywords: - 4D-STEM - electron microscopy - real-time - image processing

licensing: unknown

 task\_types:
 - Image Classification - Streamed data inference

 ai\_capability\_measured:
 - Real-time large-scale microscopy inference

 metrics:
 - Classification accuracy - Throughput

 $\begin{tabular}{lll} \bf models: & - CNN \ models \ (prototype) \\ \bf ml \ motif: & - Real-time, \ Image/CV \\ \end{tabular}$ 

type: Model

ml task: - Image Classification

solutions: 0

notes: In-progress; model design under development.

contact.name: Shuyu Qin
contact.email: shq219@lehigh.edu
results.links.name: ChatGPT LLM
fair.reproducible: in progress
fair.benchmark\_ready: False
id: d-stem
Citations: [46]

Rating	Value	Reason
dataset	2	No dataset links or FAIR metadata; unclear public access
documentation	3	Paper is clear, but lacks a GitHub repo or full reproducibility pipeline
metrics	4	Only localization accuracy and inference time mentioned; not formally benchmarked with scripts
${\bf reference\_solution}$	3	BraggNN model is described and evaluated, but no direct implementation or inference scripts available
software	2	No standalone code repository or setup instructions provided
specification	5	None



# 3.43 In-Situ High-Speed Computer Vision

Applies low-latency CNN models for image classification of plasma diagnostics streams; supports deployment on embedded platforms.

 date:
 2023-12-05

 version:
 v1.0

 last\_updated:
 2023-12

 expired:
 unknown

 valid:
 yes

 valid date:
 2023-12-05

url: https://arxiv.org/abs/2312.00128 doi: 10.48550/arXiv.2312.00128

domain: Fusion/Plasma

focus: Real-time image classification for in-situ plasma diagnostics

keywords: - plasma - in-situ vision - real-time ML

 licensing:
 Via Fermilab

 task\_types:
 - Image Classification

ai capability measured: - Real-time diagnostic inference

metrics: - Accuracy - FPS

models: - CNN

ml motif: - Real-time, Image/CV

type: Model

ml task: - Image Classification

solutions: Solution details are described in the referenced paper or repository.

notes: Embedded/deployment details in progress.

contact.name: unknown
contact.email: unknown
results.links.name: ChatGPT LLM

 $\textbf{results.links.url:} \\ \text{https://docs.google.com/document/d/1EqkRHuQs1yQqMvZs\_L6p9JAy2vKX5OCTubzttFBuRoQ/edit?usp=shared for the large of the lar$ 

fair.reproducible: in progress fair.benchmark ready: False

id: in-situ\_high-speed\_computer\_vision

Citations: [47]

### Ratings:

Rating	Value	Reason
dataset	0	Dataset not provided or described in any formal way
documentation	2	Some insight via papers, but no working repo, setup, or replication path
metrics	2	Throughput and accuracy mentioned, but not defined or benchmarked
reference_solution	1	Prototype CNNs described; no code, baseline, or training details available
software	1	No public implementation or containerized setup released
specification	3	No standardized I/O, latency constraint, or complete framing

In-Situ High-Speed Computer Vision



### 3.44 BenchCouncil AIBench

AIBench is a comprehensive benchmark suite that evaluates AI workloads at different levels (micro, component, application) across hardware systems-covering image generation, object detection, translation, recommendation, video prediction, etc.

 date:
 2020-01-01

 version:
 v1.0

 last\_updated:
 2020-01

 expired:
 unknown

 valid:
 yes

 valid date:
 2020-01-01

url: https://www.benchcouncil.org/AIBench/

**doi:** 10.48550/arXiv.1908.08998

domain: General

focus: End-to-end AI benchmarking across micro, component, and application levels

keywords: - benchmarking - AI systems - application-level evaluation

licensing: Apache License 2.0

task types: - Training - Inference - End-to-end AI workloads

ai\_capability\_measured:System-level AI workload performancemetrics:Throughput - Latency - Accuracy

models: - ResNet - BERT - GANs - Recommendation systems

 ml\_motif:
 - General

 type:
 Benchmark

 ml\_task:
 - NA

solutions: Solution details are described in the referenced paper or repository.

notes: Covers scenario-distilling, micro, component, and end-to-end benchmarks.

contact.name: Wanling Gao (BenchCouncil)

contact.email: unknown
results.links.name: ChatGPT LLM

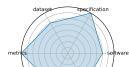
fair.reproducible: Yes fair.benchmark ready: Yes

id: benchcouncil aibench

Citations: [48]

### Ratings:

Rating	Value	Reason
dataset	3	Multiple datasets are mentioned, but not consistently FAIR-documented, versioned, or linked
documentation	3	Paper is comprehensive, but minimal user-facing documentation or structured reproduction guide
metrics	4	Metrics are appropriate, but standardization and reproducibility across tasks vary
${\bf reference\_solution}$	3	Reference models (e.g., ResNet, BERT) described; no turnkey implementation or results repository for all levels
software	3	No containerized or automated implementation provided for full benchmark suite
specification	4	Task coverage is broad and well-scoped, but system constraints and expected outputs are not uniformly defined



BenchCouncil AlBench

oference colution documentation

## 3.45 BenchCouncil BigDataBench

BigDataBench provides benchmarks for evaluating big data and AI workloads with realistic datasets (13 sources) and pipelines across analytics, graph, warehouse, NoSQL, streaming, and AI.

 date:
 2020-01-01

 version:
 v1.0

 last\_updated:
 2020-01

 expired:
 unknown

 valid:
 yes

 valid date:
 2020-01-01

url: https://www.benchcouncil.org/BigDataBench/

**doi:** 10.48550/arXiv.1802.08254

domain: General

focus: Big data and AI benchmarking across structured, semi-structured, and unstructured data

workloads

keywords: - big data - AI benchmarking - data analytics

licensing: Apache License 2.0

task\_types:
- Data preprocessing - Inference - End-to-end data pipelines
- Data processing and AI model inference performance at scale

metrics:
- Data throughput - Latency - Accuracy
models:
- CNN - LSTM - SVM - XGBoost

ml\_motif: - General type: Benchmark ml\_task: - NA

solutions: Solution details are described in the referenced paper or repository.

notes: Built on eight data motifs; provides Hadoop, Spark, Flink, MPI implementations.

contact.name: Jianfeng Zhan (BenchCouncil)

contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: benchcouncil\_bigdatabench

Citations: [49]

Rating	Value	Reason
dataset	4	Some datasets lack consistent versioning or rich metadata annotations.
documentation	4	Setup requires manual steps; some task-specific instructions lack clarity.
metrics	5	None
reference_solution	4	Not all benchmark components have fully reproducible baselines; deployment across plat-
_		forms is fragmented.
software	3	No automated setup across all tasks; some components require manual integration.
specification	4	Specific I/O formats and hardware constraints are not uniformly detailed across all tasks.





## 3.46 MLPerf HPC

MLPerf HPC introduces scientific model benchmarks (e.g., CosmoFlow, DeepCAM) aimed at large-scale HPC evaluation with >10x performance scaling through system-level optimizations.

 date:
 2021-10-20

 version:
 v1.0

 last\_updated:
 2021-10

 expired:
 unknown

 valid:
 yes

 valid date:
 2021-10-20

url: https://github.com/mlcommons/hpc

doi: 10.48550/arXiv.2110.11466

domain: Cosmology, Climate, Protein Structure, Catalysis focus: Scientific ML training and inference on HPC systems

keywords: - HPC - training - inference - scientific ML

licensing: Apache License 2.0 task types: - Training - Inference

ai capability measured: - Scaling efficiency - training time - model accuracy on HPC

metrics:
- Training time - Accuracy - GPU utilization
models:
- CosmoFlow - DeepCAM - OpenCatalyst

ml motif: - HPC/inference, HPC/training

type: Framework ml task: - NA

solutions: Solution details are described in the referenced paper or repository.

notes: Shared framework with MLCommons Science; reference implementations included.

contact.name: Steven Farrell (MLCommons)

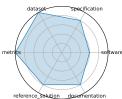
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: mlperf\_hpc
Citations: [50]

Rating	Value	Reason
dataset	5	Not all data is independently versioned or comes with standardized FAIR metadata.
documentation	4	Central guidance is available but requires domain-specific effort to replicate results across
		systems.
metrics	5	None
${\tt reference\_solution}$	4	Reproducibility and environment tuning depend on system configuration; baseline models not uniformly bundled.
software	3	Reference implementations exist but containerization and environment setup require manual effort across HPC systems.
specification	4	Hardware constraints and ${\rm I/O}$ formats are not fully defined for all scenarios.





### 3.47 MLCommons Science

MLCommons Science assembles benchmark tasks with datasets, targets, and implementations across earthquake forecasting, satellite imagery, drug screening, electron microscopy, and CFD to drive scientific ML reproducibility.

 date:
 2023-06-01

 version:
 v1.0

 last\_updated:
 2023-06

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2023-06-01

url: https://github.com/mlcommons/science

doi: unknown

domain: Earthquake, Satellite Image, Drug Discovery, Electron Microscope, CFD

focus: AI benchmarks for scientific applications including time-series, imaging, and simulation

keywords: - science AI - benchmark - MLCommons - HPC

licensing: Apache License 2.0

task types: - Time-series analysis - Image classification - Simulation surrogate modeling

ai capability measured: - Inference accuracy - simulation speed-up - generalization

metrics: - MAE - Accuracy - Speedup vs simulation

models: - CNN - GNN - Transformer

ml motif: - Time-series, Image/CV, HPC/inference

 type:
 Framework

 ml\_task:
 - NA

 solutions:
 0

notes: Joint national-lab effort under Apache-2.0 license.

contact.name: MLCommons Science Working Group

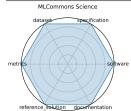
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: mlcommons science

Citations: [51]

Rating	Value	Reason
dataset	5	Public scientific datasets are used with defined splits. At least 4 FAIR principles are
		followed.
documentation	5	Thorough documentation exists covering the task, background, motivation, evaluation
		criteria, and includes a supporting paper.
metrics	5	Clearly defined metrics such as accuracy, training time, and GPU utilization are used.
		These metrics are explained and effectively capture solution performance.
reference solution	5	A reference implementation is available, well-documented, trainable/open, and includes
_		full metric evaluation and software/hardware details.
software	5	Actively maintained GitHub repository available at
		https://github.com/mlcommons/science with implementations, scripts, and repro-
		ducibility support.
specification	5	All five specification aspects are covered: system constraints, task, dataset format, bench-
-		mark inputs, and outputs.



## 3.48 LHC New Physics Dataset

A dataset of proton-proton collision events emulating a 40 MHz real-time data stream from LHC detectors, pre-filtered on electron or muon presence. Designed for unsupervised new-physics detection algorithms under latency/bandwidth constraints.

 date:
 2021-07-05

 version:
 v1.0

 last\_updated:
 2021-07

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2021-07-05

url: https://arxiv.org/pdf/2107.02157

doi: unknown

domain: Particle Physics; Real-time Triggering

focus: Real-time LHC event filtering for anomaly detection using proton collision data

keywords:
- anomaly detection - proton collision - real-time inference - event filtering - unsupervised ML

licensing: unknown

task types: - Anomaly detection - Event classification

ai capability measured: - Unsupervised signal detection under latency and bandwidth constraints

metrics: - ROC-AUC - Detection efficiency

models: - Autoencoder - Variational autoencoder - Isolation forest

 ml\_motif:
 - Multiple

 type:
 Framework

 ml\_task:
 - NA

 solutions:
 0

notes: Includes electron/muon-filtered background and black-box signal benchmarks; 1M events per

black box

contact.name: Ema Puljak (ema.puljak@cern.ch)

contact.email: unknown

datasets.links.name: Zenodo stores, background + 3 black-box signal sets. 1M events each

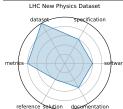
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: lhc\_new\_physics\_dataset

Citations: [52]

Rating	Value	Reason
dataset	5	Large-scale dataset hosted on Zenodo, publicly available, well-documented, with defined
		train/test structure. Appears to follow at least 4 FAIR principles.
documentation	3	Some description in papers and dataset metadata exists, but lacks a unified guide,
		README, or training setup in a central location.
metrics	4	Uses reasonable metrics (ROC-AUC, detection efficiency) that capture performance but
		lacks full explanation and standard evaluation tools.
reference solution	2	Baselines are described across multiple papers but lack centralized, reproducible imple-
_		mentations and hardware/software setup details.
software	3	While not formally evaluated in the previous version, Zenodo and paper links suggest
		available code for baseline models (e.g., autoencoders, GANs), though they are scattered
		and not unified in a single repository.
specification	3	The task and context are clearly described, but system constraints and formal in-
		puts/outputs are not fully specified.



### 3.49 MLCommons Medical AI

The MLCommons Medical AI working group develops benchmarks, best practices, and platforms (MedPerf, GaNDLF, COFE) to accelerate robust, privacy-preserving AI development for healthcare. MedPerf enables federated testing of clinical models on diverse datasets, improving generalizability and equity while keeping data onsite .

 date:
 2023-07-17

 version:
 v1.0

 last\_updated:
 2023-07

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2023-07-17

url: https://github.com/mlcommons/medical

doi: unknown

domain: Healthcare; Medical AI

focus: Federated benchmarking and evaluation of medical AI models across diverse real-world clinical

data

keywords: - medical AI - federated evaluation - privacy-preserving - fairness - healthcare benchmarks

licensing: Apache License 2.0

task types: - Federated evaluation - Model validation

ai\_capability\_measured: - Clinical accuracy - fairness - generalizability - privacy compliance

metrics:
- ROC AUC - Accuracy - Fairness metrics
models:
- MedPerf-validated CNNs - GaNDLF workflows

 ml\_motif:
 - Multiple

 type:
 Platform

 ml\_task:
 - NA

 solutions:
 0

notes: Open-source platform under Apache-2.0; used across 20+ institutions and hospitals .

contact.name: Alex Karargyris (MLCommons Medical AI)

contact.email: unknown

datasets.links.name: Multi-institutional clinical datasets, radiology

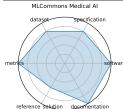
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: mlcommons medical ai

Citations: [53]

Rating	Value	Reason
dataset	4	Multi-institutional datasets used in federated settings; real-world data is handled privately onsite, but some FAIR aspects (e.g., accessibility and metadata) are implicit.
documentation	5	Extensive documentation, papers, and community support exist. Clear examples and usage instructions are provided in GitHub and publications.
metrics	5	Metrics such as ROC AUC, accuracy, and fairness are clearly specified and directly support goals like generalizability and equity.
${\bf reference\_solution}$	3	GaNDLF workflows and MedPerf-validated CNNs are referenced, but not all baseline models are centrally documented or easily reproducible.
software	5	GitHub repository (https://github.com/mlcommons/medical) provides actively maintained open-source tools like MedPerf and GaNDLF for federated medical AI evaluation.
specification	4	The platform defines federated tasks and model evaluation scenarios. Some clinical and system-level constraints are implied but not uniformly formalized across all use cases.



## 3.50 CaloChallenge 2022

The Fast Calorimeter Simulation Challenge 2022 assessed 31 generative-model submissions (VAEs, GANs, Flows, Diffusion) on four calorimeter shower datasets; benchmarking shower quality, generation speed, and model complexity .

 date:
 2024-10-28

 version:
 v1.0

 last\_updated:
 2024-10

 expired:
 unknown

 valid:
 yes

 valid date:
 2024-10-28

 url:
 http://arxiv.org/abs/2410.21611

 doi:
 10.48550/arXiv.2410.21611

 domain:
 LHC Calorimeter; Particle Physics

focus: Fast generative-model-based calorimeter shower simulation evaluation

keywords: - calorimeter simulation - generative models - surrogate modeling - LHC - fast simulation

licensing: Via Fermilab

task types: - Surrogate modeling

ai capability measured: - Simulation fidelity - speed - efficiency

metrics: - Histogram similarity - Classifier AUC - Generation latency

models: - VAE variants - GAN variants - Normalizing flows - Diffusion models

ml\_motif: - Surrogate type: Dataset

ml task: - Surrogate Modeling

solutions: Solution details are described in the referenced paper or repository.

notes: The most comprehensive survey to date on ML-based calorimeter simulation; 31 submissions

over different dataset sizes.

contact.name: Claudius Krause (CaloChallenge Lead)

contact.email: unknown

datasets.links.name: Four LHC calorimeter shower datasets

datasets.links.url: various voxel resolutions

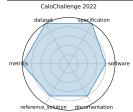
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: calochallenge\_

Citations: [54]

Rating	Value	Reason
dataset	5	Four well-structured calorimeter datasets are provided, with different voxel resolutions, open access, signal/background separation, and metadata. FAIR principles are well covered.
documentation	4	Accompanied by a detailed paper and dataset description. Reproduction of pipelines may require additional setup or familiarity with the model submissions.
metrics	5	Metrics like histogram similarity, classifier AUC, and generation latency are well defined and relevant for simulation quality, fidelity, and performance.
${\tt reference\_solution}$	4	Several baselines (GANs, VAEs, flows, diffusion models) are documented and evaluated. Some are available via community repos, though not all are fully standardized or bundled.
software	4	Community GitHub repos and model implementations are available for the 31 submissions. While not fully unified in one place, the software is accessible and reproducible.
specification	5	The task—evaluating fast generative calorimeter simulations—is clearly defined with benchmarking protocols, constraints like latency and model complexity, and structured evaluation criteria.



#### Papers With Code (SOTA Platform) 3.51

Papers With Code (PWC) aggregates benchmark suites, tasks, and code across ML research: 12,423 benchmarks, 5,358 unique tasks, and 154,766 papers with code links. It tracks SOTA metrics and fosters reproducibility.

ongoing version: v1.0 last updated: 2025-06 expired: unknown valid: yes valid date: ongoing

url: https://paperswithcode.com/sota

doi: unknown

domain: General ML; All domains

focus: Open platform tracking state-of-the-art results, benchmarks, and implementations across ML

keywords: - leaderboard - benchmarking - reproducibility - open-source

Apache License 2.0 licensing:

task types: - Multiple (Classification, Detection, NLP, etc.)

- Model performance across tasks (accuracy - F1 - BLEU - etc.)  $ai\_capability\_measured:$ 

metrics: - Task-specific (Accuracy, F1, BLEU, etc.)

models: - All published models with code

ml motif: - Multiple Platform type: ml task: - Multiple

solutions: 0

notes: Community-driven open platform; automatic data extraction and versioning.

contact.name: Papers With Code Team

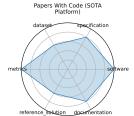
contact.email: unknown ChatGPT LLM results.links.name:

fair.reproducible: Yes fair.benchmark ready: Yes

id: papers\_with\_code\_sota\_platform

Citations:

Rating	Value	Reason
dataset	3	Relies on external datasets submitted by the community. While links are available, FAIR compliance is not guaranteed or systematically enforced across all benchmarks.
documentation	4	Strong front-end documentation and metadata on benchmarks, tasks, and models; how- ever, some benchmark-specific instructions are sparse or dependent on external paper links.
metrics	5	Tracks state-of-the-art using task-specific metrics like Accuracy, F1, BLEU, etc., with consistent aggregation and historical SOTA tracking.
${\tt reference\_solution}$	3	Provides links to implementations of many SOTA models, but no single unified reference baseline is required or maintained per benchmark.
software	5	Actively maintained open-source platform (https://paperswithcode.com) under Apache 2.0 license; includes automatic integration with GitHub, datasets, and models for reproducibility.
specification	4	Task and benchmark structures are well organized and standardized, but due to its broad coverage, input/output formats vary significantly between tasks and are not always tightly controlled.



### 3.52 Codabench

Codabench (successor to CodaLab) is a flexible, easy-to-use, reproducible API platform for hosting AI benchmarks and code-submission challenges. It supports custom scoring, inverted benchmarks, and scalable public or private queues .

 date:
 2022-01-01

 version:
 v1.0

 last\_updated:
 2025-03

 expired:
 unknown

 valid:
 yes

 valid date:
 2022-01-01

url: https://www.codabench.org/

doi: https://doi.org/10.1016/j.patter.2022.100543

domain: General ML; Multiple

focus: Open-source platform for organizing reproducible AI benchmarks and competitions

keywords: - benchmark platform - code submission - competitions - meta-benchmark

licensing: https://github.com/codalab/codalab-competitions/wiki/Privacy

task types: - Multiple

ai capability measured: - Model reproducibility - performance across datasets

metrics: - Submission count - Leaderboard ranking - Task-specific metrics

models: - Arbitrary code submissions

ml\_motif: - Multiple
type: Platform
ml\_task: - Multiple
solutions: Several

notes: Hosts 51 public competitions, ~26 k users, 177 k submissions

contact.name: Isabelle Guyon (Université Paris-Saclay)

contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes
fair.benchmark\_ready: Yes
id: codabench
Citations: [56]

Rating	Value	Reason
dataset	1	This is a platform for posting benchmarks, not a benchmark in itself.
documentation	1	This is a platform for posting benchmarks, not a benchmark in itself.
metrics	1	This is a platform for posting benchmarks, not a benchmark in itself.
reference_solution	1	This is a platform for posting benchmarks, not a benchmark in itself.
software	1	This is a platform for posting benchmarks, not a benchmark in itself.
specification	1	This is a platform for posting benchmarks, not a benchmark in itself.



# 3.53 Sabath (SBI-FAIR)

Sabath is a metadata framework from the SBI-FAIR group (UTK, Argonne, Virginia) facilitating FAIR-compliant benchmarking and surrogate execution logging across HPC systems .

 date:
 2021-09-27

 version:
 v1.0

 last\_updated:
 2023-07

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2021-09-27

url: https://sbi-fair.github.io/docs/software/sabath/

doi: unknown

domain: Systems; Metadata

focus: FAIR metadata framework for ML-driven surrogate workflows in HPC systems

keywords: - meta-benchmark - metadata - HPC - surrogate modeling

licensing: BSD 3-Clause License task types: - Systems benchmarking

ai\_capability\_measured:
 Metadata tracking - reproducible HPC workflows
 metrics:
 Metadata completeness - FAIR compliance

 models:
 - NA

 ml\_motif:
 - Systems

 type:
 Platform

 ml\_task:
 - NA

 solutions:
 0

notes: Developed by PI Piotr Luszczek at UTK; integrates with MiniWeatherML, AutoPhaseNN,

Cosmoflow, etc.

contact.name: Piotr Luszczek
contact.email: luszczek@utk.edu
results.links.name: ChatGPT LLM

 $\begin{tabular}{ll} \textbf{fair.reproducible:} & Yes \\ \textbf{fair.benchmark ready:} & N/A \\ \end{tabular}$ 

id: sabath sbi-fair

Citations: [57]

Rating	Value	Reason
dataset	4	Datasets used in surrogate benchmarks are publicly available, well-structured, and FAIR-
		aligned, but not independently hosted by Sabath itself.
documentation	3	Basic instructions and code are provided on GitHub, but more detailed walkthroughs,
		use-case examples, or tutorials are limited.
metrics	4	Emphasizes metadata completeness and FAIR compliance. Metrics are clear and well-
		matched to its metadata-focused benchmarking context.
reference_solution	3	Includes integration with multiple surrogate benchmarks and models, though not all are
_		fully documented or packaged as standardized reference solutions.
software	4	Actively maintained GitHub repository (https://github.com/icl-utk-
		edu/slip/tree/sabath) with BSD-licensed tooling for FAIR metadata capture; integrates
		with existing surrogate modeling benchmarks.
specification	4	FAIR metadata structure and logging goals are clearly described. Input/output definitions
		are implied through integrations (e.g., MiniWeatherML), though not always formalized.



### 3.54 PDEBench

PDEBench offers forward/inverse PDE tasks with large ready-to-use datasets and baselines (FNO, U-Net, PINN), packaged via a unified API. It won the SimTech Best Paper Award 2023.

 date:
 2022-10-13

 version:
 v0.1.0

 last\_updated:
 2025-05

 expired:
 unknown

 valid:
 yes

 valid date:
 2022-10-13

 ${\bf url:} \\ {\bf https://github.com/pdebench/PDEBench}$ 

 $\begin{array}{lll} \mbox{\bf doi:} & 10.48550/\mbox{arXiv.}2210.07182 \\ \mbox{\bf domain:} & \mbox{CFD; Weather Modeling} \\ \end{array}$ 

focus: Benchmark suite for ML-based surrogates solving time-dependent PDEs

keywords: - PDEs - CFD - scientific ML - surrogate modeling - NeurIPS

licensing: Other

task types: - Supervised Learning

ai capability measured: - Time-dependent PDE modeling; physical accuracy

metrics: - RMSE - boundary RMSE - Fourier RMSE

models: - FNO - U-Net - PINN - Gradient-Based inverse methods

ml\_motif: - Multiple type: Framework

ml task: - Supervised Learning

solutions: Solution details are described in the referenced paper or repository.

notes: Datasets hosted on DaRUS (DOI:10.18419/darus-2986); contact maintainers by email

contact.name: Makoto Takamoto (makoto.takamoto@neclab.eu)

contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes
fair.benchmark\_ready: Yes
id: pdebench
Citations: [58]

Rating	Value	Reason
dataset	5	Diverse PDE datasets (synthetic and real-world) hosted on DaRUS with DOIs. Datasets
		are well-documented, structured, and follow FAIR practices.
documentation	4	Strong documentation on GitHub including examples, configs, and usage instructions.
		Some model-specific details and tutorials could be further expanded.
metrics	4	Includes RMSE, boundary RMSE, and Fourier-domain RMSE. These are well-suited to
		PDE problems, though rationale behind metric choices could be expanded in some cases.
reference_solution	4	Baselines (FNO, U-Net, PINN, etc.) are available and documented, but not every model
_		includes full training and evaluation reproducibility out-of-the-box.
software	5	GitHub repository (https://github.com/pdebench/PDEBench) is actively maintained and
		includes training pipelines, data loaders, and evaluation scripts. Installation and usage
		are well-documented.
specification	5	Clearly defined tasks for forward and inverse PDE problems, with structured input/output
		formats, system constraints, and task specifications.



### 3.55 LLM-Inference-Bench

A suite evaluating inference performance of LLMs (LLaMA, Mistral, Qwen) across diverse accelerators (NVIDIA, AMD, Intel, SambaNova) and frameworks (vLLM, DeepSpeed-MII, etc.), with an interactive dashboard and per-platform metrics.

 date:
 2024-10-31

 version:
 v1.0

 last\_updated:
 2024-11

 expired:
 unknown

 valid:
 yes

 valid date:
 2024-10-31

 ${\bf url:} \hspace{1.5cm} {\bf https://github.com/argonne-lcf/LLM-Inference-Bench}$ 

doi: unknown

domain: LLM; HPC/inference

focus: Hardware performance benchmarking of LLMs on AI accelerators keywords: - LLM - inference benchmarking - GPU - accelerator - throughput

licensing: BSD 3-Clause New or Revised License

task types: - Inference Benchmarking

ai capability measured: - Inference throughput - latency - hardware utilization

metrics: - Token throughput (tok/s) - Latency - Framework-hardware mix performance

models: - LLaMA-2-7B - LLaMA-2-70B - Mistral-7B - Qwen-7B

ml motif: - HPC/inference

type: Dataset

ml task: - Inference Benchmarking

solutions: 0

notes: Licensed under BSD-3, maintained by Argonne; supports GPUs and accelerators.

contact.name: Krishna Teja Chitty-Venkata (Argonne LCF)

contact.email: unknown results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: llm-inference-bench

Citations: [59]

Rating	Value	Reason
dataset	2	No novel dataset is introduced; benchmark relies on pre-trained LLMs and synthetic
		inference inputs. Dataset structure and FAIR considerations are minimal.
documentation	4	GitHub repo provides clear usage instructions, setup guides, and interactive dashboard
		tooling. Some areas like benchmarking extensions or advanced tuning are less detailed.
metrics	5	Hardware-specific metrics (token throughput, latency, utilization) are well-defined, con-
		sistently measured, and aggregated in dashboards.
reference_solution	3	Inference configurations and baseline performance results are provided, but there are no
		full reference training pipelines or model implementations.
software	5	Public GitHub repository under BSD-3 license. Includes scripts, configurations, and dash-
		boards for running and visualizing LLM inference benchmarks across multiple accelerator
		platforms.
specification	5	Benchmark scope, models, accelerator targets, and supported frameworks are clearly spec-
		ified. Input configurations and output metrics are standardized across hardware types.



# 3.56 Delta Squared-DFT

Introduces the Delta Squared-ML paradigm-using ML corrections to DFT to predict reaction energies with accuracy comparable to CCSD(T), while training on small CC datasets. Evaluated across 10 reaction datasets covering organic and organometallic transformations.

 date:
 2024-12-13

 version:
 v1.0

 last\_updated:
 2024-12

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2024-12-13

url: https://neurips.cc/virtual/2024/poster/97788

doi: 10.48550/arXiv.2406.14347

domain: Computational Chemistry; Materials Science

focus: Benchmarking machine-learning corrections to DFT using Delta Squared-trained models for

reaction energies

keywords: - density functional theory - Delta Squared-ML correction - reaction energetics - quantum

chemistry

licensing: unknown task types: - Regression

ai\_capability\_measured:
 High-accuracy energy prediction - DFT correction
 Mean Absolute Error (eV) - Energy ranking accuracy

models: - Delta Squared-ML correction networks - Kernel ridge regression

 $\begin{tabular}{lll} $ml\_motif: & - Scientific ML \\ type: & Dataset + Benchmark \\ \end{tabular}$ 

ml task: - Regression

solutions: Solution details are described in the referenced paper or repository.

notes: Demonstrates CC-level accuracy with ~1% of high-level data. Benchmarks publicly included

for reproducibility.

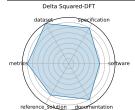
contact.name: Wei Liu
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: delta\_squared-dft

Citations: [60]

Rating	Value	Reason
dataset	4.5	Multi-modal quantum chemistry datasets are standardized and accessible; repository available.
documentation	4	Source code supports pipeline reuse, but formal evaluation splits may vary.
metrics	4	Uses standard regression metrics like MAE and energy ranking accuracy; appropriate for task.
reference solution	3.5	Includes baseline regression and kernel ridge models; implementations are reproducible.
software	3	Source code and baseline models available for ML correction to DFT; framework maturity is moderate.
specification	4	Benchmark focuses on reaction energy prediction with clear goals, though some task specifics could be formalized further.



## 3.57 Urban Data Layer (UDL)

 $\label{thm:continuous} Urban Data Layer\ standardizes\ heterogeneous\ urban\ data\ formats\ and\ provides\ pipelines\ for\ tasks\ like\ air\ quality\ prediction\ and\ land-use\ classification,\ enabling\ the\ rapid\ creation\ of\ multi-modal\ urban\ benchmarks\ .$ 

 date:
 2024-12-13

 version:
 v1.0

 last\_updated:
 2024-12

 expired:
 unknown

 valid:
 yes

 valid date:
 2024-12-13

url: https://neurips.cc/virtual/2024/poster/97837

doi: unknown

domain: Urban Computing; Data Engineering

focus:

Unified data pipeline for multi-modal urban science research
keywords:

- data pipeline - urban science - multi-modal - benchmark

licensing: unknown

task types: - Prediction - Classification

ai capability measured: - Multi-modal urban inference - standardization

metrics: - Task-specific accuracy or RMSE

models: - Baseline regression/classification pipelines

ml motif: - Data engineering

type: Framework

ml task: - Prediction, classification

solutions: 0

notes: Source code available on GitHub (SJTU-CILAB/udl); promotes reusable urban-science foun-

dation models.

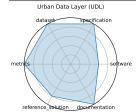
contact.name: Yiheng Wang
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: urban data layer udl

Citations: [61]

Rating	Value	Reason
dataset	5	Large, multi-modal urban datasets are open-source, well-documented, and support reproducible research.
documentation	5	GitHub repository and conference poster provide comprehensive code and reproducibility instructions.
metrics	5	Uses task-specific accuracy and RMSE metrics appropriate for prediction and classification.
${\bf reference\_solution}$	4	Baseline models available but not exhaustive; community adoption and extensions expected.
software	3	Source code is publicly available on GitHub; baseline regression and classification pipelines are included but framework maturity is moderate.
specification	5	Multiple urban science tasks like prediction and classification are well specified with clear input/output and evaluation criteria.



## 3.58 LLMs for Crop Science

Establishes a benchmark of 3,500 expert-annotated prompts and QA pairs covering crop traits, growth stages, and environmental interactions. Tests GPT-style LLMs on accuracy and domain reasoning using in-context, chain-of-thought, and retrieval-augmented prompts.

 date:
 2024-12-13

 version:
 v1.0

 last\_updated:
 2024-12

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2024-12-13

url: https://neurips.cc/virtual/2024/poster/97570

 doi:
 10.48550/arXiv.2406.03085

 domain:
 Agricultural Science; NLP

focus: Evaluating LLMs on crop trait QA and textual inference tasks with domain-specific prompts

keywords: - crop science - prompt engineering - domain adaptation - question answering

licensing: unknown

task\_types:
- Question Answering - Inference
- Scientific knowledge - crop reasoning

metrics: - Accuracy - F1 score

models: - GPT-4 - LLaMA-2-13B - T5-XXL

 ml\_motif:
 - NLP

 type:
 Dataset

 ml\_task:
 - QA, inference

solutions: Solution details are described in the referenced paper or repository.

notes: Includes examples with retrieval-augmented and chain-of-thought prompt templates; supports

few-shot adaptation.

contact.name: Deepak Patel
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: llms for crop science

Citations: [62]

#### Ratings:

Rating	Value	Reason
dataset	0	This is a model, not a benchmark.
documentation	0	This is a model, not a benchmark.
metrics	0	This is a model, not a benchmark.
reference_solution	0	This is a model, not a benchmark.
software	0	This is a model, not a benchmark.
specification	0	This is a model, not a benchmark.

LLMs for Crop Science



## 3.59 **DUNE**

Applying real-time ML methods to time-series data from DUNE detectors, exploring trigger-level anomaly detection and event selection with low latency constraints.

 date:
 2024-10-15

 version:
 v1.0

 last\_updated:
 2024-10

 expired:
 unknown

 valid:
 yes

 valid date:
 2024-10-15

 $\textbf{url:} \hspace*{2.5cm} \text{https://indico.fnal.gov/event/} 66520/\text{contributions/} 301423/\text{attachments/} 182439/250508/\text{fast\_ml\_dunedaq\_sonice} \\ \text{or } \text{and } \text{both } \text{both$ 

**doi:** 10.48550/arXiv.2103.13910

domain: Particle Physics

focus: Real-time ML for DUNE DAQ time-series data keywords: - DUNE - time-series - real-time - trigger

licensing: Via Fermilab

task types: - Trigger selection - Time-series anomaly detection

 ai\_capability\_measured:
 - Low-latency event detection

 metrics:
 - Detection efficiency - Latency

 models:
 - CNN - LSTM (planned)

 ml\_motif:
 - Real-time, Time-series

 type:
 Benchmark (in progress)

 ml\_task:
 - Supervised Learning

solutions: Solution details are described in the referenced paper or repository.

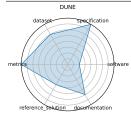
notes: Prototype models demonstrated on SONIC platform

contact.name: Andrew J. Morgan

contact.email: unknown

datasets.links.name:DUNE SONIC dataresults.links.name:ChatGPT LLMfair.reproducible:in progressfair.benchmark\_ready:Falseid:duneCitations:[63]

Rating	Value	Reason
dataset	3	Dataset lacks a public URL; FAIR metadata and versioning are missing
documentation	3	Documentation exists only in slides/GDocs; no implementation guide or structured release
metrics	4	Metrics are relevant but no benchmark baseline or detailed evaluation guidance is provided
reference_solution	2	Autoencoder prototype exists but is not reproducible; RL model still in development
software	1	Code not available; no containerization or setup provided
specification	4	Constraints like latency thresholds are described qualitatively but not numerically defined



# 3.60 MassSpecGym

 $Mass Spec Gym\ curates\ the\ largest\ public\ MS/MS\ dataset\ with\ three\ standardized\ tasks-de\ novo\ structure\ generation,\ molecule\ retrieval,\ and\ spectrum\ simulation-using\ challenging\ generalization\ splits\ to\ propel\ ML-driven\ molecule\ discovery.$ 

 date:
 2024-12-13

 version:
 v1.0

 last\_updated:
 2024-12

 expired:
 unknown

 valid:
 yes

 valid date:
 2024-12-13

url: https://neurips.cc/virtual/2024/poster/97823

doi: unknown

domain: Cheminformatics; Molecular Discovery

focus: Benchmark suite for discovery and identification of molecules via MS/MS

keywords: - mass spectrometry - molecular structure - de novo generation - retrieval - dataset

licensing: unknown

task types: - De novo generation - Retrieval - Simulation

ai\_capability\_measured:- Molecular identification and generation from spectral datametrics:- Structure accuracy - Retrieval precision - Simulation MSEmodels:- Graph-based generative models - Retrieval baselines

ml\_motif: - Benchmark

type: Dataset, Benchmark

ml task: - Generation, retrieval, simulation

solutions: 0

notes: Dataset~>1M spectra; open-source GitHub repo; widely cited as a go-to benchmark for

MS/MS tasks.

contact.name: Roman Bushuiev
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: massspecgym

Citations: [64]

Rating	Value	Reason
dataset	5	Largest public MS/MS dataset with extensive annotations; minor point deducted for lack of explicit train/validation/test splits.
documentation	1	Paper and poster describe benchmark goals and design, but documentation and user guides are minimal and repo status uncertain.
metrics	5	Well-defined metrics such as structure accuracy, retrieval precision, and simulation MSE used consistently.
${\bf reference\_solution}$	3.5	CNN-based baselines are referenced, but pretrained weights and comprehensive training pipelines are not fully documented.
software	3	Open-source GitHub repository available; baseline models and training code partially provided but overall framework maturity is moderate.
specification	5	Clearly defined tasks including molecule generation, retrieval, and spectrum simulation, scoped for MS/MS molecular identification.



# 3.61 HDR ML Anomaly Challenge (Gravitational Waves)

A benchmark for detecting anomalous transient gravitational-wave signals, including "unknown-unknowns," using preprocessed LIGO time-series at 4096 Hz. Competitors submit inference models on Codabench for continuous 50 ms segments from dual interferometers.

 date:
 2025-03-03

 version:
 v1.0

 last\_updated:
 2025-03

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2025-03-03

url: https://www.codabench.org/competitions/2626/

doi:10.48550/arXiv.2503.02112domain:Astrophysics; Time-series

focus: Detecting anomalous gravitational-wave signals from LIGO/Virgo datasets keywords: - anomaly detection - gravitational waves - astrophysics - time-series

licensing: NA

task types: - Anomaly detection

ai\_capability\_measured: - Novel event detection in physical signals

metrics:
- ROC-AUC - Precision/Recall
models:
- Deep latent CNNs - Autoencoders

ml\_motif: - Time-series type: Dataset

ml task: - Anomaly detection

solutions: Solution details are described in the referenced paper or repository.

notes: NSF HDR A3D3 sponsored; prize pool and starter kit provided on Codabench.

contact.name: HDR A3D3 Team

contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: hdr\_ml\_anomaly\_challenge\_gravitational\_waves

Citations: [65]

Rating	Value	Reason
dataset	5	Uses preprocessed LIGO/Virgo time series data at 4096 Hz, publicly available and stan-
		dard in astrophysics.
documentation	4	Documentation includes challenge instructions, starter kit details, and baseline descrip-
		tions, but could benefit from more thorough tutorials and code walkthroughs.
metrics	4	ROC-AUC, precision, and recall metrics are clearly specified and appropriate for anomaly
		detection.
reference_solution	4	Baseline deep latent CNNs and autoencoders are provided and reproducible, but not
		extensively documented.
software	4	Benchmark platform provided on Codabench with starter kits and submission infrastruc-
		ture. Code and baseline models are publicly accessible but not extensively maintained
		beyond the challenge.
specification	4	Well-defined anomaly detection task on gravitational-wave time series with clear in-
		put/output expectations and challenge constraints.



## 3.62 HDR ML Anomaly Challenge (Butterfly)

 $Image-based\ challenge\ for\ detecting\ butterfly\ hybrids\ in\ microscopy-driven\ species\ data.\ Participants\ evaluate\ models\ on\ Codabench\ using\ image\ segmentation/classification.$ 

 date:
 2025-03-03

 version:
 v1.0

 last\_updated:
 2025-03

 expired:
 unknown

 valid:
 yes

 valid date:
 2025-03-03

url: https://www.codabench.org/competitions/3764/

 $\begin{array}{lll} \mbox{\bf doi:} & 10.48550/\mbox{arXiv.}2503.02112 \\ \mbox{\bf domain:} & \mbox{Genomics; Image/CV} \\ \end{array}$ 

focus: Detecting hybrid butterflies via image anomaly detection in genomic-informed dataset

keywords: - anomaly detection - computer vision - genomics - butterfly hybrids

licensing: NA

task types: - Anomaly detection

ai\_capability\_measured:- Hybrid detection in biological systemsmetrics:- Classification accuracy - F1 scoremodels:- CNN-based detectors

 $\begin{array}{ll} \mathbf{ml\_motif:} & \quad - \mathrm{Image/CV} \\ \mathbf{type:} & \quad \mathrm{Dataset} \end{array}$ 

ml task: - Anomaly detection

solutions: Solution details are described in the referenced paper or repository.

notes: Hybrid detection benchmarks hosted on Codabench

contact.name: Imageomics/HDR Team

contact.email: unknown results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark\_ready: Yes

id: hdr\_ml\_anomaly\_challenge\_butterfly

Citations: [66]

Rating	Value	Reason
dataset	3	Dataset consists of real detector data with synthetic anomaly injections; access is re-
		stricted and requires NDA, limiting openness and FAIR compliance.
documentation	3	Challenge website provides basic descriptions and evaluation metrics but lacks compre-
		hensive tutorials or example workflows.
metrics	3	Standard metrics (ROC, F1, precision) are used; evaluation protocols are clear but not
		deeply elaborated.
reference solution	$^2$	Baselines are partially described but lack public code or reproducible execution scripts.
software	3	Codabench platform provides submission infrastructure but no fully maintained code
		repository or reproducible baseline implementations.
specification	4	Task is clearly described with domain-specific anomaly detection objectives and relevant
-		physics motivation.





## 3.63 HDR ML Anomaly Challenge (Sea Level Rise)

A challenge combining North Atlantic sea-level time-series and satellite imagery to detect flooding anomalies. Models submitted via Codabench.

 date:
 2025-03-03

 version:
 v1.0

 last\_updated:
 2025-03

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2025-03-03

url: https://www.codabench.org/competitions/3223/

**doi:** 10.48550/arXiv.2503.02112

domain: Climate Science; Time-series, Image/CV

focus: Detecting anomalous sea-level rise and flooding events via time-series and satellite imagery

keywords:
- anomaly detection - climate science - sea-level rise - time-series - remote sensing

licensing: NA

task types: - Anomaly detection

ai capability measured: - Detection of environmental anomalies

metrics:
- ROC-AUC - Precision/Recall
models:
- CNNs, RNNs, Transformers
ml motif:
- Time-series, Image/CV

type: Dataset

ml task: - Anomaly detection

solutions: Solution details are described in the referenced paper or repository.

notes: Sponsored by NSF HDR; integrates sensor and satellite data.

contact.name: HDR A3D3 Team

contact.email: unknown results.links.name: ChatGPT LLM

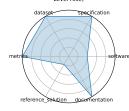
fair.reproducible: Yes fair.benchmark ready: Yes

id: hdr ml anomaly challenge sea level rise

Citations: [67]

Rating	Value	Reason
dataset	5	Uses preprocessed, public, and well-structured sensor and satellite data for the North
		Atlantic sea-level rise region.
documentation	5	Challenge page, starter kits, and related papers offer strong guidance for participants.
metrics	5	Standard metrics such as ROC-AUC, precision, and recall are specified and suitable for
		the anomaly detection tasks.
reference solution	1	No starter models or baseline implementations linked or provided publicly.
software	2	Benchmark platform exists on Codabench, but no baseline code or maintained repository
		for reference solutions provided yet.
specification	5	Well-defined anomaly detection task combining satellite imagery and time-series data,
		with clear physical and domain-specific framing.





# 3.64 Single Qubit Readout on QICK System

Implements real-time ML models for single-qubit readout on the Quantum Instrumentation Control Kit (QICK), using hls4ml to deploy quantized neural networks on RFSoC FPGAs. Offers high-fidelity, low-latency quantum state discrimination. :contentReference[oaicite:0]{index=0}

 date:
 2025-01-24

 version:
 v1.0

 last\_updated:
 2025-02

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2025-01-24

url: https://github.com/fastmachinelearning/ml-quantum-readout

 doi:
 10.48550/arXiv.2501.14663

 domain:
 Quantum Computing

focus: Real-time single-qubit state classification using FPGA firmware

keywords: - qubit readout - hls4ml - FPGA - QICK

licensing: NA

task types: - Classification

ai\_capability\_measured: - Single-shot fidelity - inference latency

metrics:
- Accuracy - Latency
models:
- hls4ml quantized NN

ml\_motif: - Real-time type: Benchmark

ml task: - Supervised Learning

solutions: Solution details are described in the referenced paper or repository.

notes: Achieves ~96% fidelity with ~32 ns latency and low FPGA resource utilization.

contact.name: Javier Campos, Giuseppe Di Guglielmo

contact.email: unknown

datasets.links.name: Zenodo: ml-quantum-readout dataset datasets.links.url: zenodo.org/records/14427490

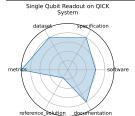
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: single\_qubit\_readout\_on\_qick\_system

Citations: [68]

Rating	Value	Reason
dataset	4	Dataset hosted on Zenodo with structured data; however, detailed documentation on
		image acquisition and labeling pipeline is limited.
documentation	4	Codabench task page and GitHub repo provide descriptions and usage instructions, but
		detailed API or deployment tutorials are limited.
metrics	5	Standard classification metrics (accuracy, latency) are used and directly relevant to the
		quantum readout task.
reference_solution	1	No baseline or starter models with runnable code are linked publicly.
software	3	Code and FPGA firmware available on GitHub; integration with hls4ml demonstrated.
		Some deployment details and examples are provided but overall software maturity is
		moderate.
specification	4	Task clearly defined: real-time single-qubit state classification with latency and fidelity
		constraints. Labeling and ground truth definitions could be more explicit.



## 3.65 GPQA: A Graduate-Level Google-Proof Question and Answer Benchmark

Contains 448 challenging questions written by domain experts, with expert accuracy at 65% (74% discounting clear errors) and non-experts reaching just 34%. GPT-4 baseline scores  $^{\sim}39\%$ -designed for scalable oversight evaluation.

 date:
 2023-11-20

 version:
 v1.0

 last\_updated:
 2023-11

 expired:
 unknown

 valid:
 yes

 valid date:
 2023-11-20

url: https://arxiv.org/abs/2311.12022 doi: 10.48550/arXiv.2311.12022

domain: Science (Biology, Physics, Chemistry)

focus: Graduate-level, expert-validated multiple-choice questions hard even with web access

keywords: - Google-proof - multiple-choice - expert reasoning - science QA

licensing: NA

task types: - Multiple choice

ai capability measured: - Scientific reasoning - knowledge probing

metrics:- Accuracymodels:- GPT-4 baselineml\_motif:- Multiple choicetype:Benchmarkml\_task:- Multiple choice

solutions: Solution details are described in the referenced paper or repository.

notes: Google-proof, supports oversight research.

contact.name: David Rein (NYU)

contact.email: unknown
datasets.links.name: GPQA dataset
datasets.links.url: zip/HuggingFace
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: gpqa\_a\_graduate-level\_google-proof\_question\_and\_answer\_benchmark

Citations: [69]

Rating	Value	Reason
dataset	5	The GPQA dataset is publicly released, well curated, with metadata and clearly documented splits.
documentation	3	Documentation includes dataset description and benchmark instructions, but lacks detailed usage tutorials or pipelines.
metrics	5	Accuracy is the primary metric and is clearly defined and appropriate for multiple-choice QA.
reference solution	1	No baseline implementations or starter code are linked or provided for reproduction.
software	3	Dataset and benchmark materials are publicly available via HuggingFace and GitHub, but no integrated runnable code or software framework is provided.
specification	5	Task is clearly defined as a multiple-choice benchmark requiring expert-level scientific reasoning. Input/output formats and evaluation criteria are well described.





### 3.66 SeafloorAI

A first-of-its-kind dataset covering 17,300 sq.km of seafloor with 696K sonar images, 827K segmentation masks, and 696K natural-language descriptions plus  $^{\sim}7M$  QA pairs-designed for both vision and language-based ML models in marine science

 date:
 2024-12-13

 version:
 v1.0

 last\_updated:
 2024-12

 expired:
 unknown

 valid:
 yes

 valid date:
 2024-12-13

url: https://neurips.cc/virtual/2024/poster/97432

doi: 10.48550/arXiv.2411.00172 domain: Marine Science; Vision-Language

focus: Large-scale vision-language dataset for seafloor mapping and geological classification

keywords: - sonar imagery - vision-language - seafloor mapping - segmentation - QA

licensing: unknown

task\_types:

ai\_capability\_measured:

metrics:

- Image segmentation - Vision-language QA

- Geospatial understanding - multimodal reasoning

- Segmentation pixel accuracy - QA accuracy

- SegFormer - ViLT-style multimodal models

ml motif: - Vision-Language

type: Dataset

ml task: - Segmentation, QA

solutions: Solution details are described in the referenced paper or repository.

notes: Data processing code publicly available, covering five geological layers; curated with marine

scientists

contact.name: Kien X. Nguyen contact.email: unknown

**datasets.links.name:** Sonar imagery + annotations

datasets.links.url: unknown
results.links.name: ChatGPT LLM
results.links.url: unknown
fair.reproducible: Yes
fair.benchmark\_ready: yes
id: seafloorai
Citations: [70]

Rating	Value	Reason
dataset	5	Large-scale, well-annotated sonar imagery dataset with segmentation masks and natural
		language descriptions; curated with domain experts.
documentation	4	Dataset description and data processing instructions are provided, but tutorials and
		benchmark usage guides are limited.
metrics	5	Standard segmentation pixel accuracy and QA accuracy metrics are clearly specified and
		appropriate for the tasks.
$reference\_solution$	4	Some baseline models (e.g., SegFormer, ViLT-style) are mentioned, but reproducible code
		or pretrained weights are not fully available yet.
software	3	Data processing code is publicly available, but no full benchmark framework or runnable
		model implementations are provided yet.
specification	5	Tasks (image segmentation and vision-language QA) are clearly defined with geospatial
		and multimodal objectives well specified.



## 3.67 SuperCon3D

SuperCon3D introduces 3D crystal structures with associated critical temperatures (Tc) and two deep-learning models: SODNet (equivariant graph model) and DiffCSP-SC (diffusion generator) designed to screen and synthesize high-Tc candidates .

 date:
 2024-12-13

 version:
 v1.0

 last\_updated:
 2024-12

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2024-12-13

url: https://neurips.cc/virtual/2024/poster/97553

doi: unknown

domain: Materials Science; Superconductivity

focus: Dataset and models for predicting and generating high-Tc superconductors using 3D crystal

structures

keywords: - superconductivity - crystal structures - equivariant GNN - generative models

licensing: unknown

task\_types:

ai\_capability\_measured:

- Regression (Tc prediction) - Generative modeling

- Structure-to-property prediction - structure generation

- MAE (Tc) - Validity of generated structures

models:- SODNet - DiffCSP-SCml\_motif:- Materials Modelingtype:Dataset + Modelsml\_task:- Regression, Generation

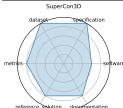
solutions:

notes: Demonstrates advantage of combining ordered and disordered structural data in model design

contact.name:Zhong Zuocontact.email:unknownresults.links.name:ChatGPT LLM

fair.reproducible: Yes
fair.benchmark\_ready: Yes
id: supercond
Citations: [71]

Rating	Value	Reason
dataset	5	Dataset contains 3D crystal structures and associated properties; well-curated but not
		fully released publicly at this time.
documentation	4	Paper and GitHub provide good metadata and data processing descriptions; tutorials and
		user guides could be expanded.
metrics	4	Metrics such as MAE for Tc prediction and validity checks for generated structures are
		appropriate and clearly described.
reference_solution	4	Paper provides model architecture details and some training insights, but no complete
		open-source reference implementations yet.
software	3	Baseline models (SODNet, DiffCSP-SC) are described in the paper; however, fully repro-
		ducible code and pretrained models are not publicly available yet.
specification	5	Tasks for regression (Tc prediction) and generative modeling with clear input/output
		structures and domain constraints are well defined.



## 3.68 GeSS

GeSS provides 30 benchmark scenarios across particle physics, materials science, and biochemistry, evaluating 3 GDL backbones and 11 algorithms under covariate, concept, and conditional shifts, with varied OOD access .

 date:
 2024-12-13

 version:
 v1.0

 last\_updated:
 2024-12

 expired:
 unknown

 valid:
 yes

 valid date:
 2024-12-13

url: https://neurips.cc/virtual/2024/poster/97816

doi: unknown

domain: Scientific ML; Geometric Deep Learning

focus: Benchmark suite evaluating geometric deep learning models under real-world distribution shifts keywords: - geometric deep learning - distribution shift - OOD robustness - scientific applications

licensing: unknown

task types: - Classification - Regression

ai\_capability\_measured:OOD performance in scientific settingsmetrics:Accuracy - RMSE - OOD robustness delta

models: - GCN - EGNN - DimeNet++

ml\_motif: - Geometric DL type: Benchmark

ml task: - Classification, Regression

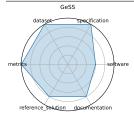
solutions: 0

notes: Includes no-OOD, unlabeled-OOD, and few-label scenarios .

contact.name: Deyu Zou
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark\_ready: Yes id: gess Citations: [72]

Rating	Value	Reason
dataset	5	Curated datasets of 3D crystal structures and material properties are included and pub-
		licly available for reproducible research.
documentation	4	Paper and poster provide solid explanation of benchmarks and scientific motivation; more
		extensive user documentation forthcoming.
metrics	5	Uses well-established metrics such as MAE and structural validity for materials modeling,
		plus accuracy and OOD robustness deltas.
reference_solution	4	Two reference models (SODNet, DiffCSP-SC) are reported with results, code expected to
		be released soon.
software	3	Reference code expected post-conference; current public software availability limited.
		Benchmark infrastructure partially described but not fully released yet.
specification	5	Benchmark clearly defines OOD robustness scenarios with classification and regression
		tasks in scientific domains, though no explicit hardware constraints are given.



# 3.69 Vocal Call Locator (VCL)

The first large-scale benchmark (767K sounds across 9 conditions) for localizing rodent vocal calls using synchronized audio and video in standard lab environments, enabling systematic evaluation of sound-source localization algorithms in bioacoustics

.

 $\begin{array}{lll} \textbf{date:} & 2024\text{-}12\text{-}13 \\ \textbf{version:} & v1.0 \\ \textbf{last\_updated:} & 2024\text{-}12 \\ \textbf{expired:} & \text{unknown} \\ \textbf{valid:} & \text{yes} \\ \textbf{valid\_date:} & 2024\text{-}12\text{-}13 \\ \end{array}$ 

url: https://neurips.cc/virtual/2024/poster/97470

doi: unknown

domain: Neuroscience; Bioacoustics

focus: Benchmarking sound-source localization of rodent vocalizations from multi-channel audio

keywords: - source localization - bioacoustics - time-series - SSL

licensing: unknown

task types: - Sound source localization

ai\_capability\_measured: - Source localization accuracy in bioacoustic settings

metrics: - Localization error (cm) - Recall/Precision

models: - CNN-based SSL models

ml\_motif: - Real-time type: Dataset

ml task: - Anomaly detection / localization

solutions: 0

notes: Dataset spans real, simulated, and mixed audio; supports benchmarking across data types .

contact.name:Ralph Petersoncontact.email:unknownresults.links.name:ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: vocal call locator vcl

Citations: [73]

Rating	Value	Reason
dataset	4	Large-scale audio dataset covering real and simulated data with standardized splits,
		though exact data formats are not fully detailed.
documentation	1	Methodology and paper are thorough, but setup instructions and runnable code are not
		publicly provided, limiting user onboarding.
metrics	5	Includes localization error, precision, recall, and other relevant metrics for robust evalu-
		ation.
reference_solution	5	Multiple baselines evaluated over diverse models and architectures, supporting repro-
		ducibility of benchmark comparisons.
software	3	Some baseline CNN models for sound source localization are reported, but no publicly
		available or fully integrated runnable codebase yet.
specification	5	Well-defined localization tasks with multiple scenarios and real-world environment con-
		ditions; input/output formats clearly described.



# 3.70 SPIQA (LLM)

A workshop version of SPIQA comparing 10 LLM adapter methods on the SPIQA benchmark with scientific diagram/questions. Highlights performance differences between chain-of-thought and end-to-end adapter models.

 date:
 2024-12-13

 version:
 v1.0

 last\_updated:
 2024-12

 expired:
 unknown

 valid:
 yes

 valid date:
 2024-12-13

url: https://neurips.cc/virtual/2024/poster/97575

doi: 10.48550/arXiv.2407.09413

domain: Multimodal Scientific QA; Computer Vision

focus: Evaluating LLMs on image-based scientific paper figure QA tasks (LLM Adapter performance)

keywords: - multimodal QA - scientific figures - image+text - chain-of-thought prompting

licensing: unknown

task types: - Multimodal QA

ai capability measured: - Visual reasoning - scientific figure understanding

metrics: - Accuracy - F1 score

models: - LLaVA - MiniGPT-4 - Owl-LLM adapter variants

solutions: Solution details are described in the referenced paper or repository.

notes: Companion to SPIQA main benchmark; compares adapter strategies using same images and

QA pairs.

contact.name: Xiaoyan Zhong contact.email: unknown results.links.name: ChatGPT LLM

fair.reproducible: Yes
fair.benchmark\_ready: Yes
id: spiqa\_llm
Citations: [74]

Rating	Value	Reason
dataset	5	Full dataset available on Hugging Face with train/test/valid splits.
documentation	5	Full paper available
metrics	4	Reports accuracy and F1; fair but no visual reasoning-specific metric.
reference solution	4	10 LLM adapter baselines; results included without constraints.
software	5	Well-documented codebase available on Github
specification	3.5	Task of QA over scientific figures is sufficient but not fully formalized in input/output
-		terms. No hawrdware constraints.



## 3.71 The Well

A 15 TB collection of ML-ready physics simulation datasets (HDF5), covering 16 domains-from biology to astrophysical magnetohydrodynamic simulations-with unified API and metadata. Ideal for training surrogate and foundation models on scientific data

 date:
 2024-12-03

 version:
 v1.0

 last\_updated:
 2025-06

 expired:
 unknown

 valid:
 yes

 valid\_date:
 2024-12-03

**url:** https://polymathic-ai.org/the\_well/

doi: unknown

 domain:
 biological systems, fluid dynamics, acoustic scattering, astrophysical MHD

 focus:
 Foundation model + surrogate dataset spanning 16 physical simulation domains

keywords: - surrogate modeling - foundation model - physics simulations - spatiotemporal dynamics

licensing: BSD 3-Clause License task types: - Supervised Learning

ai\_capability\_measured: - Surrogate modeling - physics-based prediction

metrics:- Dataset size - Domain breadthmodels:- FNO baselines - U-Net baselinesml\_motif:- Foundation model, Surrogate

1

type: Dataset

ml task: - Supervised Learning

solutions:

notes: Includes unified API and dataset metadata; see 2025 NeurIPS paper for full benchmark details.

Size: 15 TB.

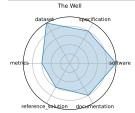
contact.name: Ruben Ohana

contact.email:rohana@flatironinstitute.orgdatasets.links.name:16 simulation datasetsdatasets.links.url:HDF5) via PyPI/GitHub

results.links.name: ChatGPT LLM

fair.reproducible: Yes
fair.benchmark\_ready: Yes
id: the\_well
Citations: [75]

Rating	Value	Reason
dataset	5	15 TB of ML-ready HDF5 datasets across 16 physics domains. Public, well-structured,
		richly annotated, and designed with FAIR principles in mind.
documentation	4	The GitHub repo and NeurIPS paper provide detailed guidance on dataset use, structure,
		and training setup. Tutorials and walkthroughs could be expanded further.
metrics	3	Domain breadth and dataset size are emphasized. Standardized quantitative metrics for
		model evaluation (e.g., RMSE, accuracy) are not uniformly applied across all domains.
$reference\_solution$	3	Includes FNO and U-Net baselines, but does not yet provide fully trained, reproducible
		models or scripts across all datasets.
software	5	BSD-licensed software and unified API are available via GitHub and PyPI. Supports
		loading and manipulating large HDF5 datasets across 16 domains.
specification	4	The benchmark includes clearly defined surrogate modeling tasks, data structure, and
		metadata. However, constraints and formal task specs vary slightly across domains.



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