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/ML Mo-	AI Capabil-	Metrics	Models		g c itation
						tif	ity			Rat- ing	
ClimateLearn - Weather Forcasting dataset - The Climate Company of the Company of	ClimateLearr - Weather Forcasting	Climate & Earth Science	ML for weather and climate model- ing	medium- range forecast- ing, ERA5, data- driven	Forecasting	Sequence Predic- tion/Forecasting	Global weather g prediction (3-5 days)	RMSE, Anomaly correla- tion	CNN base- lines, ResNet variants	5.00	[1]
ClimateLeam - Downscaling dataset - Downscal	ClimateLearr Down-scaling	ı Climate & Earth Science	ML for weather and climate model- ing	medium- range forecast- ing, ERA5, data- driven	Forecasting	Regression	Global weather prediction (3-5 days)	RMSE, Anomaly correla- tion	CNN base- lines, ResNet variants	5.00	[1]
ClimateLearn - Climate Projection Projection dataset The Climate Projection dataset The Clima	ClimateLearr - Climate Projection	n Climate & Earth Science	ML for weather and climate model- ing	medium- range forecast- ing, ERA5, data- driven	Forecasting	Regression	Global weather prediction (3-5 days)	RMSE, Anomaly correla- tion	CNN base- lines, ResNet variants	5.00	[1]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat-	g c itation
										ing	
MLCommons Science - Cloudid dataset Types (feation metrics - Shidion downmentation - Shidion - Shidion downmentation - Shidion - Shidion - Shidion downmentation - Shidion - S	* MLCommons Science - CloudMask	Climate & Earth Science	AI benchmarks for scientific applications including timeseries, imaging, and simulation	science AI, bench- mark, MLCom- mons, HPC	Time-series analysis, Image clas- sification, Simulation surrogate modeling	Classification	Inference accuracy, simulation speed-up, generalization	MAE, Accu- racy, Speedup vs simu- lation	CNN, GNN, Trans- former	5.00	[2]
MLCommons Science - Earthquidals - Types (feation processes) - Types (feation processe	MLCommons Science - Earth- quake	Climate & Earth Science	AI benchmarks for scientific applications including timeseries, imaging, and simulation	science AI, benchmark, MLCommons, HPC	Time-series analysis, Image clas- sification, Simulation surrogate modeling	Sequence Predic- tion/Forecasting	Inference accuracy, g simulation speed-up, generalization	MAE, Accu- racy, Speedup vs simu- lation	CNN, GNN, Trans- former	5.00	[2]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo-	AI Capabil-	Metrics	Models	Avera	gcCitation
						tif	ity			Rat- ing	
MLCommons Science - Candle to data to the second se	MLCommons Science - Candle UNO	Biology & Medicine	AI benchmarks for scientific applications including timeseries, imaging, and simulation	science AI, benchmark, MLCommons, HPC	Time-series analysis, Image clas- sification, Simulation surrogate modeling	Classification	Inference accuracy, simulation speed-up, generalization	MAE, Accu- racy, Speedup vs simu- lation	CNN, GNN, Trans- former	5.00	[2]
MLCommons Science - STEM dataset The ification metrics reference SALIO downfeetable	MLCommons Science - STEMDL	Materials Science	AI bench- marks for sci- entific appli- cations includ- ing time- series, imaging, and sim- ulation	science AI, bench- mark, MLCom- mons, HPC	Time-series analysis, Image clas- sification, Simulation surrogate modeling	Classification	Inference accuracy, simulation speed-up, generalization	MAE, Accu- racy, Speedup vs simu- lation	CNN, GNN, Trans- former	5.00	[2]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	geCitation
ARC.Challenge (Advanced Reasoning Challenge) dataset Specification metrics reference Soldion dosementation	* ARC- Challenge (Advanced Reasoning Challenge)	Computat: Science & AI	io (Callade- school science with rea- soning empha- sis	grade- school, science QA, chal- lenge set, reasoning	Multiple choice	Reasoning & Generaliza- tion	Commonsense and scientific reasoning	Accuracy	GPT-4, Claude	4.83	[3]
MOLGEN datassa progression metrics reference skullo documentation	MOLGEN	Chemistry	Molecular genera- tion and opti- mization	SELFIES, GAN, property optimiza- tion	Distribution learning, Goal-oriented generation	Generative	Generation of valid and optimized molecular structures	Validity%, Nov- elty%, QED, Docking score, penal- ized logP	MolGen	4.83	[4]
Open Graph Benchmark (OGB Biology dalaysa profifeation metrics	Open Graph Benchmark (OGB) - Biology	Biology & Medicine	Biological graph property predic- tion	node prediction, link prediction, graph classification	Node property prediction, Link property prediction, Graph property prediction	Sequence Predic- tion/Forecastin	Scalability and gener- g alization in graph ML for biology	Accuracy, ROC- AUC	GCN, Graph- SAGE, GAT	4.83	[5]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	g c itation
LLMs for Crop Science datassa The first in the control of the cont	LLMs for Crop Science	Climate & Earth Science	Evaluating LLMs on crop trait QA and textual inference tasks with domain-specific prompts	crop science, prompt en- gineering, domain adap- tation, question answering	Question Answering, Inference	Reasoning & Generalization	Scientific knowledge, crop reason- ing	Accuracy, F1 score	GPT- 3.5, GPT-4, Claude- 3-opus, Qwen- max, LLama3- 8B, InternLM2 7B, Qwen1.5- 7B	4.67	[6]
metris	e SciCode	Computati Science & AI	o Sal entific code genera- tion and problem solving	code synthesis, scientific computing, programming benchmark	Coding	Generative	Program synthesis, scientific computing	Solve rate (%)	Claude3.5- Sonnet	4.50	[7]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo-	AI Capabil- ity	Metrics	Models	Avera Rat-	gCitation
						611	ity			ing	
Calochallenge 2022 datage The Readon metric reference skallen goarmentatio	CaloChalleng	e High Energy Physics	Fast generative- model- based calorime- ter shower simu- lation evalua- tion	calorimeter simulation, generative models, surrogate modeling, LHC, fast simulation	Surrogate modeling	Generative	Simulation fidelity, speed, efficiency	Histogram similarity, Classifier AUC, Generation latency	VAE variants, GAN variants, Normal- izing flows, Diffu- sion models	4.50	[8]
PDEBench datage The effection metrics reference you tipe governmentation	PDEBench	Computati Science & AI, Climate & Earth Science, Mathe- matics	oilednchmark suite for ML- based surro- gates solving time- dependent PDEs	CPDEs, CFD, scientific ML, surrogate modeling, NeurIPS	Supervised Learning	Regression	Time- dependent PDE model- ing; physical accuracy	RMSE, bound- ary RMSE, Fourier RMSE	FNO, U-Net, PINN, Gradient- Based inverse methods	4.50	[9]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo-	AI Capabil-	Metrics	Models	Avera	gcCitatio
_						tif	ity			Rat- ing	
Urban Data Layer (UDJ PMZ) Concentration Prediction data set the Concentration Prediction metrics reference Totalism governmentation	Turban Data Layer (UDL) PM2.5 Concentration Prediction	Climate & Earth Science	Unified data pipeline for multimodal urban science research	data pipeline, urban science, multi- modal, benchmark	Prediction, Classification	Regression	Multi-modal urban in- ference, standardiza- tion	Task- specific accu- racy or RMSE	Baseline regres- sion/classi pipelines	4.50 fication	[10]
Urban Daha Layer (UDA)- Bullit up Area Classification dulasgas- The decador reference, Seation governmentalic	Urban Data Layer (UDL) Built-up Area Clas- sification	Climate & Earth Science	Unified data pipeline for multimodal urban science research	data pipeline, urban science, multi- modal, benchmark	Prediction, Classification	Classification	Multi-modal urban in- ference, standardiza- tion	Task- specific accu- racy or RMSE	Baseline regres- sion/classi pipelines	4.50 fication	[10]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo-	AI Capabil-	Metrics	Models	Avera	gcCitation
						tif	ity			Rat- ing	
Urban Data Layer (UDL) - Administrative Boundings identification data see	Urban Data Layer (UDL) - Administrative Boundaries Identification	Climate & Earth Science	Unified data pipeline for multimodal urban science research	data pipeline, urban science, multi- modal, benchmark	Prediction, Classification	Classification	Multi-modal urban in- ference, standardiza- tion	Task- specific accu- racy or RMSE	Baseline regres- sion/classif pipelines	4.50 fication	[10]
urban Data Layer (UD) El Nino Anomaly Detection Nino Anomaly Detection adaptate the state of	Urban Data Layer (UDL) El Nino Anomaly Detection	Climate & Earth Science	Unified data pipeline for multimodal urban science research	data pipeline, urban science, multi- modal, benchmark	Prediction, Classification	Anomaly Detection	Multi-modal urban in- ference, standardiza- tion	Task- specific accu- racy or RMSE	Baseline regres- sion/classif pipelines	4.50 fication	[10]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	gCitation
SPIQA (LLM) datasse— specification metrics reference souldo dowmentatio	SPIQA (LLM)	Computati Science & AI	io Falaluating 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	Multimodal Reasoning	Visual reasoning, scientific figure understanding	Accuracy, F1 score	LLaVA, MiniGPT- 4, Owl- LLM adapter variants	4.42	[11]
MLCommons Medical AI - Pancress Segmentation (OPC dataset of the common	MLCommons Medical AI - Pancreas Segmen- tation (DFCI)	Biology & Medicine	Federated bench- marking and evalua- tion of medi- cal AI models across diverse real- world clinical data	medical AI, federated evaluation, privacy- preserving, fairness, healthcare bench- marks	Federated evaluation, Model valida- tion	Classification	Clinical accuracy, fairness, generalizability, privacy compliance	ROC AUC, Accu- racy, Fairness metrics	MedPerf-validated CNNs, GaN-DLF work-flows	4.33	[12]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	gCitation
MiCommons Medical Al. Brai Tumor Segmentation (Brait) dataset Type Redor	* MLCommons Medical AI - Brain Tumor Segmen- tation (BraTS)	s Biology & Medicine	Federated bench- marking and evalua- tion of medi- cal AI models across diverse real- world clinical data	medical AI, federated evaluation, privacy- preserving, fairness, healthcare bench- marks	Federated evaluation, Model valida- tion	Classification	Clinical accuracy, fairness, generalizability, privacy compliance	ROC AUC, Accu- racy, Fairness metrics	MedPerf- validated CNNs, GaN- DLF work- flows	4.33	[12]
MLCommons Medical Al- Surgical Workflow Phase Necognition (Surgh) (Lube) datase reference medical reference medical reference medical	MLCommons Medical AI - Surgical Workflow Phase Recog- nition (SurgML- Cube)	s Biology & Medicine	Federated bench- marking and evalua- tion of medi- cal AI models across diverse real- world clinical data	medical AI, federated evaluation, privacy- preserving, fairness, healthcare bench- marks	Federated evaluation, Model valida- tion	Classification	Clinical accuracy, fairness, generalizability, privacy compliance	ROC AUC, Accu- racy, Fairness metrics	MedPerf-validated CNNs, GaN-DLF work-flows	4.33	[12]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	g c itation
seafloarial datased the final or metrics and t	SeafloorAI	Climate & Earth Science	Large-scale vision- language dataset for seafloor mapping and ge- ological classifi- cation	sonar imagery, vision- language, seafloor mapping, segmen- tation, QA	Image seg- mentation, Vision- language QA	Classification	Geospatial understand- ing, mul- timodal reasoning	Segmentat pixel ac- curacy, QA accuracy	ioßegFormer ViLT- style multi- modal models	, 4.33	[13]
Seafloor Genal datasset The fication metrics reference selection documentals	SeafloorGen	AIClimate & Earth Science	Large-scale vision- language dataset for seafloor mapping and ge- ological classifi- cation	sonar imagery, vision- language, seafloor mapping, segmen- tation, QA	Image seg- mentation, Vision- language QA	Reasoning & Generalization	Geospatial understand- ing, mul- timodal reasoning	Segmentat pixel ac- curacy, QA accuracy	ioSegFormer ViLT- style multi- modal models		[13]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo-	AI Capabil- ity	Metrics	Models	Avera Rat-	gCitation
										ing	
reference rolution dosermentali	* GeSS - Track Pileup	High Energy Physics	Benchmar's uite evaluating geometric deep learning models under realworld distribution shifts	k geometric deep learn- ing, dis- tribution shift, OOD robustness, scientific applica- tions	Classification	Classification	OOD performance in scientific settings	Accuracy, RMSE, OOD ro- bustness delta	GCN, EGNN, DimeNet+	4.33 +	[14]
GeSS - Track Signal data sale track Signal da	GeSS - Track Signal	High Energy Physics		k geometric deep learn- ing, dis- tribution shift, OOD robustness, scientific applica- tions	Classification	Classification	OOD performance in scientific settings	Accuracy, RMSE, OOD ro- bustness delta	GCN, EGNN, DimeNet+	4.33 +	[14]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	gCitation
GBSS - DrugODD datassa The fination metrics reference 764dion dosementation	GeSS - DrugOOD	Biology & Medicine	Benchmarl suite evaluating geometric deep learning models under realworld distribution shifts	deep learning, distribution shift, OOD robustness, scientific applications	Classification	Classification	OOD performance in scientific settings	Accuracy, RMSE, OOD ro- bustness delta	GCN, EGNN, DimeNet+	4.33	[14]
reference soldion governmentation	GeSS - QMOF	Materials Science	Benchmarl suite evaluating geometric deep learning models under realworld distribution shifts	deep learning, distribution shift, OOD robustness, scientific applications	Classification, Regression	Regression	OOD performance in scientific settings	Accuracy, RMSE, OOD ro- bustness delta	GCN, EGNN, DimeNet+	4.33	[14]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Rat-	gcitation
OCP (Open Catalyst Project) datasset The flication metrics reference 3644(on downmentation	OCP (Open Catalyst Project)	Chemistry Mate- rials Science	Catalyst adsorption energy prediction	DFT re- laxations, adsorption energy, graph neural networks	Energy prediction, Force prediction	Regression	Prediction of adsorption energies and forces	MAE (en- ergy), MAE (force)	CGCNN, SchNet, DimeNet+ GemNet- OC	4.17 +-,	[15]- [18]
Jet Classification dataset The Theatreation metrics reference Solution downmentation	Jet Classification	High Energy Physics	Real- time classifi- cation of parti- cle jets using HL-LHC simu- lation features	classification, real-time ML, jet tagging, QKeras	Classification	Classification	Real-time inference, model com- pression performance	Accuracy, AUC	Keras DNN, QKeras quan- tized DNN	4.17	[19]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	gCitation
regulat Sensor Data Compression dataset specification dataset spec	Irregular Sensor Data Com- pression	High Energy Physics	Real- time com- pression of sparse sensor data with autoen- coders	compression, autoen- coder, sparse data, ir- regular sampling	Compression	Generative	Reconstruction quality, com- pression efficiency	MSE, Com- pression ratio	Autoencod Quan- tized autoen- coder		[20]
MLPerf HPC - DeepCAM	MLPerf HPC - Cosmoflow	High Energy Physics	Scientific ML training and in- ference on HPC systems	HPC, training, inference, scientific ML	Training, Inference	Regression	Scaling efficiency, training time, model ac- curacy on HPC	Training time, Accuracy, GPU utilization	CosmoFlow Deep- CAM, Open- Catalyst	v,4.17	[21]
MLPert HPC - DeepCAM datasase	MLPerf HPC - DeepCAM	Climate & Earth Science	Scientific ML training and in- ference on HPC systems	HPC, training, inference, scientific ML	Training, Inference	Classification	Scaling efficiency, training time, model ac- curacy on HPC	Training time, Accuracy, GPU utilization	DeepCAM		[21]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	geCitatio
MJPM* HPC. Open Catalyst Project DimeNet ++ dataspt The first open Catalyst metrics	MLPerf HPC - Open Catalyst Project DimeNet++	Chemistry	Scientific ML training and in- ference on HPC systems	HPC, training, inference, scientific ML	Training, Inference	Regression	Scaling efficiency, training time, model ac- curacy on HPC	Training time, Accuracy, GPU utilization	DeepCAM		[21]
MLPerf HPC - OpenFold dataset	MLPerf HPC - OpenFold	Biology & Medicine	Scientific ML training and in- ference on HPC systems	HPC, training, inference, scientific ML	Training, Inference	Sequence Predic- tion/Forecastin	Scaling efficiency, g training time, model ac- curacy on HPC	Training time, Accuracy, GPU utilization	DeepCAM	4.17	[21]
HDR ML Anonally Challenge Gravitational Waves and Adaptive Challenge Gravitational Waves and Adaptive Challenge Chal	" HDR ML Anomaly Challenge - Gravi- tational Waves	High Energy Physics	Detecting anomalous gravitation wave signals from LIGO/Virg datasets	waves, astrophysics, time-series	Anomaly Detection	Anomaly Detection	Novel event detection in physical signals	ROC- AUC, Preci- sion/Recal	Deep latent CNNs, l Autoen- coders	4.17	[22]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	gCitation
SuperCon3D. Property Prediction dataset The fication dataset The fication downfentaling reference solution downfentaling downfen	SuperCon3D - Property Prediction	Materials Science	Dataset and models for pre- dicting and gen- erating high-Tc super- con- ductors using 3D crystal struc- tures	superconduct crystal structures, equivari- ant GNN, generative models	ivRegression (Tc prediction), Generative modeling	Regression	Structure- to-property prediction, structure generation	MAE (Tc), Validity of gen- erated struc- tures	SODNet, DiffCSP- SC	4.17	[23]
SuperCon3D - Inverse Crist Structure Generalis Tructure Generalis	SuperCon3D - Inverse Crystal Structure Generation	Materials Science	Dataset and models for pre- dicting and gen- erating high-Tc super- con- ductors using 3D crystal struc- tures	superconduct crystal structures, equivari- ant GNN, generative models	iv Reg ression (Tc prediction), Generative modeling	Generative	Structure- to-property prediction, structure generation	MAE (Tc), Validity of gen- erated struc- tures	SODNet, DiffCSP- SC	4.17	[23]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	gCitatio
BalsBench (Biological Al Scientist Benchmark) - Guestion Answering datases - The Control of the	BaisBench (Biolog- ical AI Scientist Bench- mark) - Question Answering	Biology & Medicine	Omics- driven AI re- search tasks	single-cell anno- tation, biological QA, au- tonomous discovery	Cell type annotation, Multiple choice	Reasoning & Generalization	Autonomous biological research capabilities	Annotation accuracy, QA accuracy	n LLM- based AI scientist agents	4.00	[24]
Busigners (tillologisal A) Scientis Benefitmants - Cell Type Annotation datasses - Type Anestation datasses - Type Annotation reference Switten - doserferintation	BaisBench (Biolog- ical AI Scientist Bench- mark) - Cell Type Annotation	Biology & Medicine	Omics- driven AI re- search tasks	single-cell anno- tation, biological QA, au- tonomous discovery	Cell type annotation, Multiple choice	Classification	Autonomous biological research capabilities	Annotation accuracy, QA accuracy	based AI scientist agents	4.00	[24]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	g c itation
The Well datases the control of the	The Well	Biology & Medicine, Compu- tational Science & AI, High Energy Physics	Foundation model + sur- rogate dataset span- ning 16 physical simu- lation domains	n surrogate modeling, foundation model, physics simula- tions, spatiotem- poral dynamics	Supervised Learning	Sequence Predic- tion/Forecasting	Surrogate modeling, g physics-based prediction	Dataset size, Domain breadth	FNO base- lines, U-Net baselines	4.00	[25]
MMU Massive Mulitask Language Understanding) datasas The dicatio metrical metrical datasas The dicatio	MMLU (Massive Multitask Language Under- standing)	Computat Science & AI	ionAdademic knowl- edge and rea- soning across 57 subjects	multitask, multiple- choice, zero-shot, few-shot, knowledge probing	Multiple choice	Reasoning & Generaliza- tion	General reasoning, subject- matter under- standing	Accuracy	GPT-40, Gem- ini 1.5 Pro, o1, DeepSeek- R1	3.83	[26]
SatingNet datasas metrica metrica reference 3-skutton governmentati	SatImgNet	Climate & Earth Science	Satellite imagery classifi- cation	land-use, zero-shot, multi-task	Image classification	Multimodal Reasoning	Zero-shot land-use classification	Accuracy	CLIP, BLIP, ALBEF	3.83	[27]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo-	AI Capabil- ity	Metrics	Models	Avera Rat-	g c itation
						011	Toy			ing	
reference solution downfeentation	* GPQA Di- amond	Biology & Medicine, Chem- istry, High Energy Physics	Graduate- level scientific reason- ing	Google- proof, graduate- level, sci- ence QA, chemistry, physics	Multiple choice, Multi- step QA	Reasoning & Generaliza- tion	Scientific reasoning, deep knowledge	Accuracy	o1, DeepSeek- R1	3.83	[28]
PRMSOOK dataget Type(fication metrics reference, houseon documentation	PRM800K	Mathemat	icsMath rea- soning general- ization	calculus, algebra, number theory, geometry	Problem solving	Reasoning & Generaliza- tion	Math reasoning and generalization	Accuracy	GPT-4	3.83	[29]
FEABroch (Rinke Element Analysis Benchmark): Evaluating Linguage Modes of Multiphysics Reasoning Ability dataset metric reference_volutiondosementation	FEABench (Finite Element Analysis Bench- mark): Evaluating Language Models on Mul- tiphysics Reasoning Ability	Mathemat	icsFEA simu- lation accuracy and perfor- mance	finite element, simulation, PDE	Simulation, Performance evaluation	Reasoning & Generaliza- tion	Numerical simulation accuracy and efficiency	Solve time, Error norm	FEniCS, deal.II	3.83	[30]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	gCitation
Neural Actificature Catelagi for Fast Physics Applications dataset psecification dataset psecification metric pseudoja dagoermentation dagoermentation	Neural Architecture Codesign for Fast Physics Applications	High Energy Physics	Automated neural architecture search and hardware-efficient model codesign for fast physics applications	I neural architecture search, FPGA deployment, quantization, pruning, hls4ml	Classification, Peak finding	Classification	Hardware- aware model optimization; low-latency inference	Accuracy, Latency, Re- source utiliza- tion	NAC- based Brag- gNN, NAC- optimized Deep Sets (jet)	3.83	[31]
Delto Squared-DFT datassat Type-(Reation metrical reference, totaliza dissementation	Delta Squared- DFT	Chemistry Mate- rials Science	Benchmarl machine- learning correc- tions to DFT using Delta Squared- trained models for re- action energies	cinlensity functional theory, Delta Squared- ML cor- rection, reaction energetics, quantum chemistry	Regression	Regression	High- accuracy energy pre- diction, DFT correction	Mean Absolute Error (eV), Energy ranking accuracy	Delta Squared- ML correc- tion net- works, Kernel ridge re- gression	3.83	[32]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	gCitation
HDR ML Anomaty Challenge - S Level Risie datassa— Specification metrical datassa— Specification reference Solution governmentation	HDR ML Anomaly Challenge - Sea Level Rise	Climate & Earth Science	Detecting anomalous sea-level rise and flooding events via timeseries and satellite imagery	anomaly detection, climate science, sea-level rise, time- series, remote sensing	Anomaly Detection	Anomaly Detection	Detection of environmen- tal anomalies	ROC- AUC, Preci- sion/Recal	CNNs, RNNs, Trans- l formers	3.83	[33]
Vocal Call Locator (VCL) dataset The Rection metrics reference_Solution_stourmentation	Vocal Call Locator (VCL)	Biology & Medicine		kingurce lo- calization, bioa- coustics, time-series, SSL	Sound source localization	Regression	Source lo- calization accuracy in bioacoustic settings	Localization error (cm), Recall/Precis	based SSL models	3.83	[34]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	gCitation
MassSpecKym - De novo molec generation dataset - specification dataset - speci	MassSpecGyr - De novo molecule generation	${ m mChemistry}$	Benchmarl suite for discov- ery and identifi- cation of molecules via MS/MS	c mass spec- trometry, molecular structure, de novo generation, retrieval, dataset	De novo generation, Retrieval, Simulation	Generative	Molecular identification and gener- ation from spectral data	Structure accu- racy, Re- trieval preci- sion, Simu- lation MSE	Graph- based gener- ative models, Re- trieval baselines	3.75	[35]
MassSpecCym - Molecule Retrieval daisus - Types (feation	* MassSpecGyr - Molecule Retrieval	${ m nChemistry}$	Benchmark suite for discov- ery and identifi- cation of molecules via MS/MS	c mass spec- trometry, molecular structure, de novo generation, retrieval, dataset	De novo generation, Retrieval, Simulation	Regression	Molecular identification and gener- ation from spectral data	Structure accu- racy, Re- trieval preci- sion, Simu- lation MSE	Graph- based gener- ative models, Re- trieval baselines	3.75	[35]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo-	AI Capabil-	Metrics	Models	Avera	gcitatio
_				-		tif	ity			Rat- ing	
MassSpecCym - Spectrum invalidation dataget - Spectrum invalid	MassSpecGy - Spectrum Simulation	${ m mChemistry}$	Benchmarl suite for discov- ery and identifi- cation of molecules via MS/MS	c mass spectrometry, molecular structure, de novo generation, retrieval, dataset	De novo generation, Retrieval, Simulation	Regression	Molecular identification and gener- ation from spectral data	Structure accu- racy, Re- trieval preci- sion, Simu- lation MSE	Graph- based gener- ative models, Re- trieval baselines	3.75	[35]
SPIOA (Scientific Paper Imag Question Answering) datasea procedure of the Commentary metrics of the Commentary of the Co	SPIQA (Scientific Paper Image Question Answering)	Computat: Science & AI	io M illtimoda QA on scientific figures	al multimodal QA, figure under- standing, table com- prehension, chain-of- thought	Question answering, Multimodal QA, Chain- of-Thought evaluation	Multimodal Reasoning	Visual- textual reasoning in scientific contexts	Accuracy, F1 score	Chain- of- Thought models, Multi- modal QA systems	3.67	[36]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo-	AI Capabil-	Metrics	Models		g c itation
						tif	ity			Rat- ing	
GPQA: A Graduate Level Coop Proof Description and Answer Benchmark dataset Type (feator reference Type (feator MedQA	GPQA: A Graduate- Level Google- Proof Ques- tion and Answer Benchmark	Biology & Medicine, High Energy Physics, Chem- istry	Graduate-level, expert-validated multiple-choice questions hard even with web access	Google- proof, multiple- choice, expert reasoning, science QA	Multiple choice	Reasoning & Generalization	Scientific reasoning, knowledge probing	Accuracy	GPT-4 baseline	3.67	[37]
MedQA dalagat Tspecification metrics metrics metrics reference, Tolutton documentati	e MedQA	Biology & Medicine	Medical board exam QA	USMLE, diagnos- tic QA, medical knowledge, multilin- gual	Multiple choice	Reasoning & Generaliza- tion	Medical diagnosis and knowledge retrieval	Accuracy	Neural reader, Retrieval- based QA systems	3.50	[38]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	g C itation
Single Qubit Readout on Qid System disasses Sy	Single Qubit Readout on QICK System	Computati Science & AI	olRedal- time single- qubit state classifi- cation using FPGA firmware	qubit readout, hls4ml, FPGA, QICK	Classification	Classification	Single-shot fi- delity, infer- ence latency	Accuracy, Latency	hls4ml quan- tized NN	3.50	[39]
CFOBench (Fluid Dynamics datasa) Specification of the control of t	c CFDBench (Fluid Dynamics)	Mathemat	icsNeural operator surro- gate model- ing	neural opera- tors, CFD, FNO, DeepONet	Surrogate modeling	Regression	Generalization of neural op- erators for PDEs	L2 error, MAE	FNO, Deep- ONet, U-Net	3.33	[40]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	g c itatior
CURIE (Scientific Long Conte Understanding, Ressoning and Information Extraction) dataset production dataset production	CURIE (Scientific Long- Context Under- standing, Reasoning and In- formation Extrac- tion)	Materials Science, High Energy Physics, Biology & Medicine, Chemistry, Climate & Earth Science	Long- context scientific reason- ing	long- context, infor- mation extraction, multi- modal	Information extraction, Reasoning, Concept tracking, Aggregation, Algebraic manipulation, Multimodal comprehen- sion	Reasoning & Generaliza- tion	Long-context understand- ing and scientific reasoning	Accuracy	unkown	3.33	[41]
Smart Poets for LHC datases Transferation metals for LHC datases Transferation reference_Solution_dasementals	Smart Pixels for LHC	High Energy Physics	On- sensor, in-pixel ML fil- tering for high- rate LHC pixel de- tectors	smart pixel, on- sensor inference, data re- duction, trigger	Image Classification, Data filtering	Classification	On-chip, low-power in- ference; data reduction	Data rejection rate, Power per pixel	2-layer pixel NN	3.33	[42]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	g c itation
LHC New Physics Dataset dataset Specification people and the service of the servi	LHC New Physics Dataset	High Energy Physics	Real- time LHC event filter- ing for anomaly detec- tion using proton collision data	anomaly detection, proton collision, real-time inference, event fil- tering, unsuper- vised ML	Anomaly Detection, Event classification	Anomaly Detection	Unsupervised signal detection under latency and bandwidth constraints	ROC- AUC, Detec- tion effi- ciency	Autoencoo Varia- tional autoen- coder, Isolation forest	ieß.33	[43]
Quantum Computing Benchma (OML) datages The Clication metries reference southin dissementation	Quantum Computing Bench- marks (QML)	Computat Science & AI	io Quantum algo- rithm perfor- mance evalua- tion	quantum circuits, state prepara- tion, error correction	Circuit benchmark- ing, State classification	Classification	Quantum algorithm performance and fidelity	Fidelity, Success proba- bility	IBM Q, IonQ, AQT@LB!	3.17 NL	[44]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	g c itation
Ultrafast jet classification at the HL-HC dataset the HL-HC datase	Ultrafast jet clas- sification at the HL-LHC	High Energy Physics	FPGA- optimized real- time jet origin classifi- cation at the HL-LHC	jet classification, FPGA, quantization- aware training, Deep Sets, Interaction Networks	Classification	Classification	Real-time inference under FPGA constraints	Accuracy, Latency, Re- source utiliza- tion	MLP, Deep Sets, Inter- action Network	3.17	[45]
HEDM (BraggNN) dataset The floation metrics reference_bellion_tourmentation	HEDM (BraggNN)	Materials Science	Fast Bragg peak analysis using deep learn- ing in diffrac- tion mi- croscopy	BraggNN, diffrac- tion, peak finding, HEDM	Peak detection	Classification	High- throughput peak localiza- tion	Localization accuracy, Inference time	nBraggNN	3.17	[46]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo-	AI Capabil-	Metrics	Models	Avera	geCitatio:
J				, and the second		tif	ity			Rat- ing	
ADSTEM datasat Transferation metrics reference_Totalion_documentali	sotware or 4D-STEM	Materials Science	Real- time ML for scanning trans- mission electron mi- croscopy	4D-STEM, electron mi- croscopy, real-time, image processing	Image Classification, Streamed data inference	Classification	Real-time large-scale microscopy inference	Classificati ac- curacy, Through- put	io©NN models (proto- type)	3.17	[47]
Beam Control dataspat The Circuit Control metroc. Southon documentati	Beam Control	High Energy Physics	Reinforcer learning control of accel- erator beam position	neRfL, beam stabi- lization, control systems, simulation	Control	Reinforcement Learn- ing/Control	Policy performance in simulated accelerator control	Stability, Control loss	DDPG, PPO (planned)	3.00	[48], [49]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	gCitation
Intelligent experiments through real-time Al dataset Types (Facility and Intelligent Control of the Control of	Intelligent exper- iments through real-time	High Energy Physics	Real- time FPGA- based trigger- ing and detector con- trol for sPHENIX and fu- ture EIC	FPGA, Graph Neural Network, hls4ml, real-time inference, detector control	Trigger classification, Detector control, Real- time inference	Classification	Low-latency GNN in- ference on FPGA	Accuracy (charm and beauty detec- tion), Latency (mi- cros), Re- source uti- lization (LUT/FF)	Bipartite Graph Network with Set Trans- formers (BGN- ST), GarNet (edge- classifier)	3.00	[50]
HOR ML Anomaly Challenge Butterfly dataset The Circulor and the Control of the Co	HDR ML Anomaly Challenge - Butterfly	Biology & Medicine	Detecting hybrid butter- flies via image anomaly detec- tion in genomic- informed dataset	anomaly detection, computer vision, genomics, butterfly hybrids	Anomaly Detection	Anomaly Detection	Hybrid detection in biological systems	Classificati accu- racy, F1 score	ocNN- based detec- tors	3.00	[51]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo- tif	AI Capabil- ity	Metrics	Models	Avera Rat- ing	g c itation
datasel The fication datasel reference solution documentation	DUNE	High Energy Physics	Real- time ML for DUNE DAQ time- series data	DUNE, time-series, real-time, trigger	Trigger selection, Time-series anomaly detection	Anomaly Detection	Low-latency event detec- tion	Detection effi- ciency, Latency	CNN, LSTM (planned)	2.83	[52]
FrontierMath dataset The (fication) reference 3-Nation docemental)	FrontierMath	Mathemat	icChallengin ad- vanced mathe- matical reason- ing	g symbolic reasoning, number theory, algebraic geometry, category theory	Problem solving	Reasoning & Generalization	Symbolic and abstract mathematical reasoning	Accuracy	unknown	2.50	[53]
AIME (American Invitational Mathematics Examinational Mathematics Examinational Mathematics (American Invitational Mathematics) (American	AIME (American Invita- tional Mathe- matics Examina- tion)	Mathemat	icsPre- college ad- vanced problem solving	algebra, combi- natorics, number theory, geometry	Problem solving	Reasoning & Generalization	Mathematical problem- solving and reasoning	Accuracy	unknown	2.33	[54]

Ratings	Name	Domain	Focus	Keywords	Task Types	AI/ML Mo-	AI Capabil- ity	Metrics	Models	Avera Rat-	gCitation
						UII	Ity			ing	
Quench detection datapad The Relation metrics reference 3044100 governmentalis	Quench detection	High Energy Physics	Real- time detec- tion of super- con- ducting magnet quenches using ML	quench detection, autoen- coder, anomaly detection, real-time	Anomaly Detection, Quench local- ization	Anomaly Detection	Real-time anomaly de- tection with multi-modal sensors	ROC- AUC, Detec- tion latency	Autoencood RL agents (in develop- ment)	e 2 .17	[55]
Materials Project datassal specification metrical specification reference solution downferentation	* Materials Project	Materials Science	DFT- based property predic- tion	DFT, materials genome, high- throughput	Property pre- diction	Regression	Prediction of inorganic ma- terial proper- ties	MAE, R^2	Automatm Crystal Graph Neural Net- works	.inle:9,2	[56]
In-Situ High-Speed Compute Vision dataset The Indiana	In-Situ High- Speed Computer Vision	High Energy Physics	Real- time image classifi- cation for in- situ plasma diagnos- tics	plasma, insitu vision, real-time ML	Image Classification	Classification	Real-time diagnostic inference	Accuracy, FPS	CNN	1.50	[57]

2 Radar Chart Table

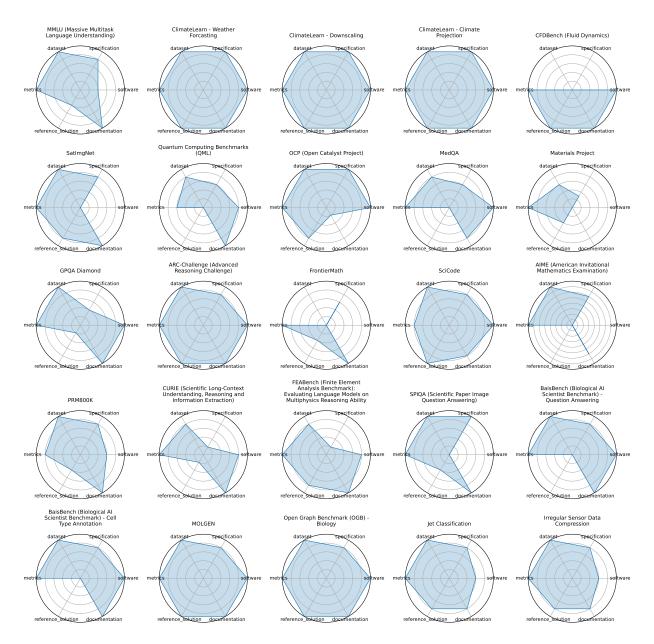


Figure 1: Radar chart overview (page 1)

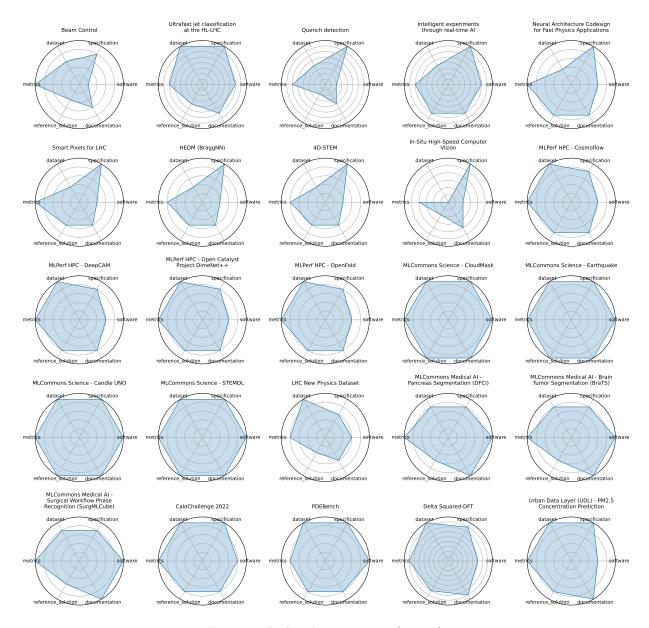


Figure 2: Radar chart overview (page 2)

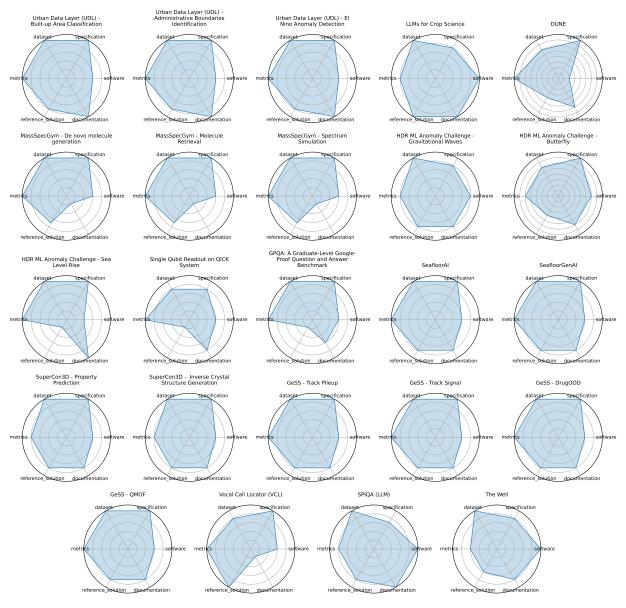


Figure 3: Radar chart overview (page 3)

3 Benchmark Details

3.1 ClimateLearn - Weather Forcasting

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 & Earth Science

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:
 - Sequence Prediction/Forecasting

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

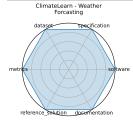
results.links.name: ClimateLearn Paper (results section) results.links.url: https://arxiv.org/abs/2307.01909

fair.reproducible: Yes fair.benchmark ready: Yes

id: climatelearn_-_weather_forcasting

Citations: [1]

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	5	A Quickstart notebook is provided that uses ResNet as a baseline model
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.



3.2 ClimateLearn - Downscaling

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 & Earth Science

focus: ML for weather and climate modeling

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

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

ml_motif: - Regression 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

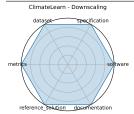
results.links.name: ClimateLearn Paper (results section) results.links.url: https://arxiv.org/abs/2307.01909

fair.reproducible: Yes fair.benchmark ready: Yes

id: climatelearn_-_downscaling

Citations: [1]

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	5	A Quickstart notebook is provided that uses ResNet as a baseline model
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.



3.3 ClimateLearn - Climate Projection

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 & Earth Science

focus: ML for weather and climate modeling

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

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

ml_motif: - Regression 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

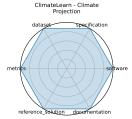
results.links.name: ClimateLearn Paper (results section) results.links.url: https://arxiv.org/abs/2307.01909

fair.reproducible: Yes fair.benchmark ready: Yes

id: climatelearn_-_climate_projection

Citations: [1]

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	5	A Quickstart notebook is provided that uses ResNet as a baseline model
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.



3.4 MLCommons Science - CloudMask

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:
 no

 valid:
 yes

 valid date:
 2023-06-01

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

 $\begin{array}{lll} \mbox{\bf doi:} & 10.1007/978\text{-}3\text{-}031\text{-}23220\text{-}6_4 \\ \mbox{\bf domain:} & - \mbox{Climate \& Earth Science} \\ \end{array}$

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: - Classification
type: Framework
ml_task: - NA
solutions: 0

 notes:
 Joint effort under Apache-2.0 license.

 contact.name:
 MLCommons Science Working Group

 contact.email:
 science-chairs@mlcommons.org

datasets.links.name: CANDLE UNO

datasets.links.url: https://github.com/mlcommons/science/tree/main/benchmarks/uno#data-description

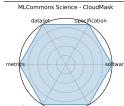
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark_ready: Yes

id: mlcommons_science_-_cloudmask

Citations: [2]

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-
specification	0	mark inputs, and outputs.



3.5 MLCommons Science - Earthquake

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:
 no

 valid:
 yes

 valid_date:
 2023-06-01

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

 doi:
 10.1007/978-3-031-23220-6_4

 domain:
 - Climate & Earth Science

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:
- Sequence Prediction/Forecasting

 type:
 Framework

 ml_task:
 - NA

 solutions:
 0

 notes:
 Joint effort under Apache-2.0 license.

 contact.name:
 MLCommons Science Working Group

 contact.email:
 science-chairs@mlcommons.org

datasets.links.name: CANDLE UNO

datasets.links.url: https://github.com/mlcommons/science/tree/main/benchmarks/uno#data-description

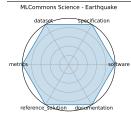
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: mlcommons_science_-_earthquake

Citations: [2]

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-
specification	0	mark inputs, and outputs.
		mark inputs, and outputs.



3.6 MLCommons Science - Candle UNO

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:
 no

 valid:
 yes

 valid date:
 2023-06-01

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

 $\begin{array}{lll} \mbox{\bf doi:} & 10.1007/978\text{-}3\text{-}031\text{-}23220\text{-}6_4 \\ \mbox{\bf domain:} & - \mbox{Biology \& Medicine} \\ \end{array}$

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: - Classification
type: Framework
ml_task: - NA
solutions: 0

 notes:
 Joint effort under Apache-2.0 license.

 contact.name:
 MLCommons Science Working Group

 contact.email:
 science-chairs@mlcommons.org

datasets.links.name: CANDLE UNO

datasets.links.url: https://github.com/mlcommons/science/tree/main/benchmarks/uno#data-description

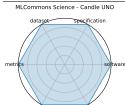
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: mlcommons_science_-_candle_uno

Citations: [2]

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.



3.7 MLCommons Science - STEMDL

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:
 no

 valid:
 yes

 valid date:
 2023-06-01

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

doi: 10.1007/978-3-031-23220-6_4

domain: - Materials Science

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:
 - Classification

 type:
 Framework

 ml_task:
 - NA

 solutions:
 0

 notes:
 Joint effort under Apache-2.0 license.

 contact.name:
 MLCommons Science Working Group

 contact.email:
 science-chairs@mlcommons.org

datasets.links.name: A Database of Convergent Beam Electron Diffraction Patterns for Machine Learning of the

Structural Properties of Materials

datasets.links.url: https://doi.ccs.ornl.gov/dataset/7aed61eb-e44c-5b14-82ea-07917d1b2d3b

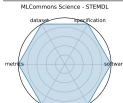
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: mlcommons_science_-_stemdl

Citations: [2]

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.



3.8 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:
 10.48550/arXiv.1803.05457

 domain:
 - Computational Science & AI

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

 $ml_motif:$ - Reasoning & Generalization

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: ARC-Solvers

results.links.url: https://github.com/allenai/arc-solvers

fair.reproducible: Yes fair.benchmark ready: Yes

id: arc-challenge _advanced _reasoning _challenge

Citations: [3]

Rating	Value	Reason
dataset	5	Data accessible, offers instructions on how to download the data via CLI tools. Splits
		provided on Huggingface
documentation	5	Explains all necessary information inside a paper
metrics	5	All questions in the dataset are multiple choice, all have a correct answer
reference solution	5	Reference solution is available and containerized
software	5	Code is available and well documented for evaluation.
specification	4	Task is clear and inputs/outputs are provided along with format on dataset card.





3.9 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: 2024-12-17

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: - Chemistry

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

licensing: MIT License

task_types:

ai_capability_measured:
metrics:

- Distribution learning - Goal-oriented generation
- Generation of valid and optimized molecular structures
- Validity% - Novelty% - QED - Docking score - penalized logP

models:
- MolGen
ml_motif:
- Generative
type:
Benchmark

ml task: - Supervised Learning

solutions: 0

notes:

contact.name: zhangningyu@zju.edu.cn

contact.email: Ningyu Zhang

 datasets.links.name:
 MolGen: A Pre-trained Molecular Language Model

 datasets.links.url:
 https://github.com/zjunlp/MolGen/tree/main

results.links.name: Domain-Agnostic Molecular Generation with Chemical Feedback

results.links.url: https://arxiv.org/abs/2301.11259

fair.reproducible: Yes
fair.benchmark_ready: Yes
id: molgen
Citations: [4]

Rating	Value	Reason
dataset	5	Dataset and train/test splits are available through the github repo, as well as mentions
		of source datasets in the paper.
documentation	5	All necessary information is provided in the paper and github repo
metrics	5	Metrics are well defined and appropriate for the task
reference_solution	5	A pretrained model is provided, as well as training code and instructions
software	5	Code is available on the github repo, along with instructions to run the model and repro-
		duce results.
specification	4	Task, datset format, and input/output formats are well specified. No system constraints
		are mentioned.



3.10 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:
 - Biology & Medicine

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

metrics:
- Accuracy - ROC-AUC
models:
- GCN - GraphSAGE - GAT
ml motif:
- Sequence Prediction/Forecasting

type: Benchmark

ml task: - Supervised Learning

solutions: 0

notes: Community-driven updates

contact.name: OGB Team contact.email: ogb@cs.stanford.edu

datasets.links.name: ogb@cs.stanford.edu
OGB Webpage

datasets.links.url: https://ogb.stanford.edu/docs/dataset_overview/

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

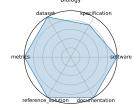
id: open_graph_benchmark_ogb_-_biology

Citations: [5]

Ratings:

Rating	Value	Reason
dataset	5	Fully FAIR- datasets are versioned, split, and accessible via a standardized API; extensive
		metadata and documentation are included.
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.
reference solution	5	Multiple baselines implemented and documented (GCN, GAT, GraphSAGE).
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; splits are well-defined.

Open Graph Benchmark (OGB) Biology



3.11 LLMs for Crop Science

Establishes a benchmark of over 5000 expert-annotated QA pairs and prompts in Chinese and English, 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:
 2024-11-13

 version:
 v1.0

 last_updated:
 2024-11

 expired:
 unknown

 valid:
 yes

 valid_date:
 2024-11-13

url: https://openreview.net/forum?id=hMj6jZ6JWU#discussion

doi: N/A

domain: - Climate & Earth Science

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: CC-BY-NC-4.0

task_types:
- Question Answering - Inference
- Scientific knowledge - crop reasoning

metrics: - Accuracy - F1 score

models: - GPT-3.5 - GPT-4 - Claude-3-opus - Qwen-max - LLama3-8B - InternLM2-7B - Qwen1.5-7B

ml motif: - Reasoning & Generalization

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

datasets.links.name: CROP Benchmark (Test Split)

datasets.links.url: https://huggingface.co/datasets/AI4Agr/CROP-benchmark

results.links.name: Empowering and Assessing the Utility of Large Language Models in Crop Science - Experiments

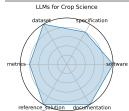
results.links.url: https://renqichen.github.io/The Crop/

fair.reproducible: Yes fair.benchmark ready: Yes

id: llms_for_crop_science

Citations: [6]

Rating	Value	Reason
dataset	5	Dataset adheres to all FAIR principles, is well-documented, and publicly available on
		Hugging Face. Train/Test splits are provided across two Huggingface datasets.
documentation	5	The benchmark is well documented with a detailed paper, README, and webpage.
		Instructions for reproducing results are clear.
metrics	4	Accuracy is mentioned in the README and webpage as an evaluation metric,
${\bf reference_solution}$	5	A reference solution is available and well documented. Training code is provided for multiple open weight models.
software	5	Code for evaluation and training of multiple models is available and well documented.
		Environment details are provided.
specification	4	Tasks are clearly defined (QA, inference) with structured input/output formats, though no system constraints are provided.



3.12 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://scicode-bench.github.io/
doi: 10.48550/arXiv.2407.13168
domain: - Computational Science & AI

focus: Scientific code generation and problem solving

keywords: - code synthesis - scientific computing - programming benchmark

licensing: unknown task types: - Coding

ai capability measured: - Program synthesis, scientific computing

metrics:
- Solve rate (%)
- Claude3.5-Sonnet
ml_motif:
- Generative
type:
- Benchmark

ml task: - Supervised Learning

solutions:unknownnotes:Goodcontact.name:Minyang Tiancontact.email:mtian8@illinois.edudatasets.links.name:SciCode on Huggingface

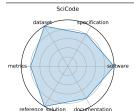
datasets.links.url: https://huggingface.co/datasets/SciCode1/SciCode

results.links.name: SciCode Learderboard

results.links.url: https://scicode-bench.github.io/leaderboard/

fair.reproducible: Yes
fair.benchmark_ready: Yes
id: scicode
Citations: [7]

Rating	Value	Reason
dataset	5	Dataset meets all FAIR principles, test and validation splits are available (no train split)
documentation	4	Paper containing all needed info except for evaluation criteria
metrics	4	Metrics stated, grading guidelines are provided in repo (problems are pass/fail)
${\tt reference_solution}$	5	Code to evaluate is available and well documented. Baseline models include closed and open weight models
software	5	Code to run exists on github repo
specification	4	Expected outputs and broad types of inputs stated. Few details on output grading. No HW constraints.



3.13 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:
 - High Energy 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: - Generative 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

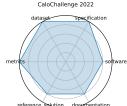
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: calochallenge_

Citations: [8]

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.
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 submis-
		sions. 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.



3.14 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

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

 ${\bf doi:} \hspace{1.5cm} 10.48550/{\rm arXiv.2210.07182}$

 domain:
 - Computational Science & AI - Climate & Earth Science - Mathematics

 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: - Regression type: Framework

ml task: - Supervised Learning

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

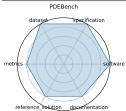
notes: Datasets hosted on DaRUS (DOI:10.18419/darus-2986); contact maintainers by email

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: [9]

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.



3.15 Urban Data Layer (UDL) - PM2.5 Concentration Prediction

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

 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: - Climate & Earth Science

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: - Regression 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

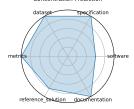
fair.reproducible: Yes fair.benchmark ready: Yes

id: urban data layer udl - pm concentration prediction

Citations: [10]

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.





3.16 Urban Data Layer (UDL) - Built-up Area Classification

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

 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: - Climate & Earth Science

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: - Classification type: Framework

ml task: - Prediction, classification

solutions: 0

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

dation models.

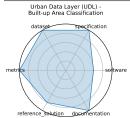
contact.name: Yiheng Wang
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: urban data layer udl - built-up area classification

Citations: [10]

Rating	Value	Reason
dataset	5	Large, multi-modal urban datasets are open-source, well-documented, and support repro-
		ducible 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 classifica-
		tion.
${\tt reference_solution}$	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
Software	Ü	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.



3.17 Urban Data Layer (UDL) - Administrative Boundaries Identification

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

 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: - Climate & Earth Science

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: - Classification type: Framework

ml task: - Prediction, classification

solutions: 0

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

dation models.

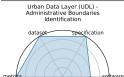
contact.name: Yiheng Wang
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: urban data layer udl - administrative boundaries identification

Citations: [10]

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.



reference solution documentation

3.18 Urban Data Layer (UDL) - El Nino Anomaly Detection

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

 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: - Climate & Earth Science

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: - Anomaly Detection

type: Framework

ml task: - Prediction, classification

solutions: 0

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

dation models.

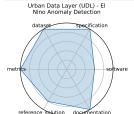
contact.name: Yiheng Wang
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: urban_data_layer_udl_-_el_nino_anomaly_detection

Citations: [10]

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.



3.19 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:
 - Computational Science & AI

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

ml motif: - Multimodal Reasoning

type: Benchmark
ml task: - Multimodal QA

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: [11]

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.



3.20 MLCommons Medical AI - Pancreas Segmentation (DFCI)

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:
 10.1038/s42256-023-00652-2

 domain:
 - Biology & Medicine

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:
 - Classification

 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_-_pancreas_segmentation_dfci

Citations: [12]

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 sup-
		port goals like generalizability and equity.
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 main-
		tained 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.



3.21 MLCommons Medical AI - Brain Tumor Segmentation (BraTS)

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

 $\begin{array}{lll} \mbox{\bf doi:} & 10.1038/s42256\text{-}023\text{-}00652\text{-}2 \\ \mbox{\bf domain:} & - \mbox{Biology \& Medicine} \\ \end{array}$

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:
 - Classification

 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 - brain tumor segmentation brats

Citations: [12]

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 sup-
		port goals like generalizability and equity.
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 main-
		tained 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.



3.22 MLCommons Medical AI - Surgical Workflow Phase Recognition (SurgMLCube)

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

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

 $_{
m data}$

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:
 - Classification

 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

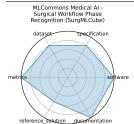
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: mlcommons_medical_ai_-__surgical_workflow_phase_recognition_surgmlcube

Citations: [12]

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.



3.23 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:
 - Climate & Earth Science

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: - Classification 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

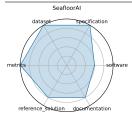
scientists

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: [13]

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.



3.24 SeafloorGenAI

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:
 - Climate & Earth Science

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: - Reasoning & Generalization

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: seafloorgenai

Citations: [13]

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.



3.25 GeSS - Track Pileup

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: - High Energy Physics

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

ai_capability_measured:OOD performance in scientific settingsAccuracy - RMSE - OOD robustness delta

models: - GCN - EGNN - DimeNet++

ml_motif: - Classification 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_-_track_pileup

Citations: [14]

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.



3.26 GeSS - Track Signal

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: - High Energy Physics

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

ai_capability_measured:OOD performance in scientific settingsmetrics:Accuracy - RMSE - OOD robustness delta

models: - GCN - EGNN - DimeNet++

ml_motif: - Classification type: Benchmark

ml task: - Classification, Regression

solutions: 0

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

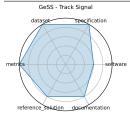
contact.name: Deyu Zou
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: gess_-_track_signal

Citations: [14]

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.



3.27 GeSS - DrugOOD

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: - Biology & Medicine

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

ai_capability_measured:OOD performance in scientific settingsAccuracy - RMSE - OOD robustness delta

models: - GCN - EGNN - DimeNet++

ml_motif: - Classification type: Benchmark

ml task: - Classification, Regression

solutions: 0

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

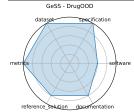
contact.name: Deyu Zou
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: gess_-_drugood

Citations: [14]

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.



$3.28 \quad GeSS - QMOF$

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: - Materials Science

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

 ${\bf models:} \qquad \qquad {\bf - GCN - EGNN - DimeNet} + +$

ml_motif: - Regression type: Benchmark

ml task: - Classification, Regression

solutions: 0

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

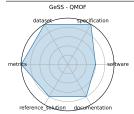
contact.name: Deyu Zou
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: gess_-_qmof

Citations: [14]

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.



3.29 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: - Regression type: Benchmark

ml task: - Supervised Learning

solutions: 0

notes: Public leaderboards; active community development

contact.name: unknown contact.email: unknown datasets.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

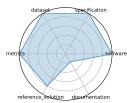
fair.reproducible: Yes fair.benchmark ready: Yes

id: ocp_open_catalyst_project

Citations: [15], [16], [17], [18]

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.





3.30 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

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

 $\begin{array}{lll} \textbf{doi:} & 10.48550/\mathrm{arXiv.2207.07958} \\ \textbf{domain:} & - \text{High Energy Physics} \end{array}$

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: - Classification 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

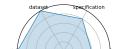
datasets.links.url: https://zenodo.org/record/6619768

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

id: jet classification

Citations: [19]

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
Jet Classification		



70

3.31 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:
 - High Energy 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: - Generative 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

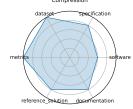
fair.reproducible: Yes fair.benchmark ready: Yes

id: irregular_sensor_data_compression

Citations: [20]

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





3.32 MLPerf HPC - Cosmoflow

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

 $\begin{array}{lll} \mbox{\bf doi:} & 10.48550/\mbox{arXiv.}2110.11466 \\ \mbox{\bf domain:} & -\mbox{High Energy Physics} \end{array}$

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: - Regression 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_-_cosmoflow

Citations: [21]

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.
	_	ÿ.
metrics	5	None
$reference_solution$	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 I/O formats are not fully defined for all scenarios.





3.33 MLPerf HPC - DeepCAM

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:
 - Climate & Earth Science

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:
- DeepCAM
ml_motif:
- Classification
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

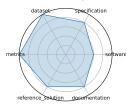
fair.reproducible: Yes fair.benchmark ready: Yes

id: mlperf_hpc_-_deepcam

Citations: [21]

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
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 I/O formats are not fully defined for all scenarios.





3.34 MLPerf HPC - Open Catalyst Project DimeNet++

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: - Chemistry

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:
- DeepCAM
ml_motif:
- Regression
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_-_open_catalyst_project_dimenet_

Citations: [21]

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
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 I/O formats are not fully defined for all scenarios.





3.35 MLPerf HPC - OpenFold

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

 $\begin{array}{lll} \mbox{\bf doi:} & 10.48550/\mbox{arXiv.}2110.11466 \\ \mbox{\bf domain:} & -\mbox{Biology \& Medicine} \\ \end{array}$

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: - DeepCAM

ml motif: - Sequence Prediction/Forecasting

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_-_openfold

Citations: [21]

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
$reference_solution$	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 I/O formats are not fully defined for all scenarios.





3.36 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/

 $\begin{array}{lll} \mbox{\bf doi:} & 10.48550/\mbox{arXiv.}2503.02112 \\ \mbox{\bf domain:} & -\mbox{High Energy Physics} \\ \end{array}$

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: - Anomaly Detection

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: [22]

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.



3.37 SuperCon3D - Property Prediction

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

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:
 - Regression (Tc prediction) - Generative modeling

 ai_capability_measured:
 - Structure-to-property prediction - structure generation

metrics: - MAE (Tc) - Validity of generated structures

models:
- SODNet - DiffCSP-SC
ml motif:
- Regression

ml_motif: - Regression type: Dataset + Models ml_task: - Regression, Generation

solutions:

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

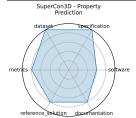
contact.name:Zhong Zuocontact.email:unknownresults.links.name:ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: supercond_-_property_prediction

Citations: [23]

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.



3.38 SuperCon3D - Inverse Crystal Structure Generation

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

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:
 - Regression (Tc prediction) - Generative modeling

 ai_capability_measured:
 - Structure-to-property prediction - structure generation

metrics:
- MAE (Tc) - Validity of generated structures
models:
- SODNet - DiffCSP-SC

ml_motif: - Generative type: Dataset + Models

ml_task: - Regression, Generation solutions: 0

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

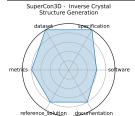
contact.name:Zhong Zuocontact.email:unknownresults.links.name:ChatGPT LLM

fair.reproducible: Yes fair.benchmark_ready: Yes

id: supercond _- _ inverse _crystal _structure _generation

Citations: [23]

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.



3.39 BaisBench (Biological AI Scientist Benchmark) - Question Answering

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

 $\begin{array}{lll} \textbf{url:} & & \text{https://arxiv.org/abs/2505.08341} \\ \textbf{doi:} & & 10.48550/\text{arXiv.2505.08341} \\ \textbf{domain:} & & - \text{Biology \& Medicine} \\ \end{array}$

focus: 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:
- Reasoning & Generalization

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

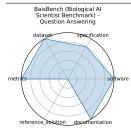
datasets.links.url: https://github.com/EperLuo/BaisBench

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

id: baisbench_biological_ai_scientist_benchmark_-_question_answering

Citations: [24]

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.



3.40 BaisBench (Biological AI Scientist Benchmark) - Cell Type Annotation

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/2505.08341

 doi:
 10.48550/arXiv.2505.08341

 domain:
 - Biology & Medicine

focus: 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: - Almotation accuracy - QA acc models: - LLM-based AI scientist agents

ml_motif: - Classification 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

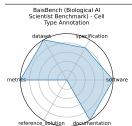
datasets.links.url: https://github.com/EperLuo/BaisBench

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

id: baisbench_biological_ai_scientist_benchmark_-_cell_type_annotation

Citations: [24]

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.



3.41 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:- Biology & Medicine - Computational Science & AI - High Energy Physicsfocus: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:- Sequence Prediction/Forecasting

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. "Benchmarks" are nominally baseline models that were trained on different parts

of the dataset, all of them being time series prediction tasks.

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: [25]

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.



3.42 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://huggingface.co/datasets/cais/mmlu

 doi:
 10.48550/arXiv.2009.03300

 domain:
 - Computational Science & AI

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-40 - Gemini 1.5 Pro - o1 - DeepSeek-R1

ml motif: - Reasoning & Generalization

type: Benchmark

ml task: - Supervised Learning

solutions: 1 notes: Good

contact.name: Dan Hendrycks
contact.email: dan (at) safe.ai
datasets.links.name: Huggingface Dataset

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

results.links.name: Measuring Massive Multitask Language Understanding - Test Leaderboard results.links.url: https://github.com/hendrycks/test?tab=readme-ov-file#test-leaderboard

fair.reproducible: Yes fair.benchmark ready: Yes

d: mmlu_massive_multitask_language_understanding

Citations: [26]

	** 1	
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	2	Some code is available on github to reproduce results via OpenAI API, but not well
		documented
specification	4	No system constraints



reference solution documentation

3.43 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://satinbenchmark.github.io/
doi: 10.48550/arXiv.2304.11619
domain: - Climate & Earth Science
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: - Multimodal Reasoning

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

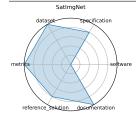
datasets.links.url: https://huggingface.co/datasets/jonathan-roberts1/SATIN

results.links.name: SatImgNet Leaderboard

results.links.url: https://satinbenchmark.github.io/ pages/leaderboard/

fair.reproducible: Yes
fair.benchmark_ready: Yes
id: satimgnet
Citations: [27]

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.



3.44 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: - Biology & Medicine - Chemistry - High Energy Physics

focus: Graduate-level scientific reasoning

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

licensing: unknown

task_types:
Multiple choice - Multi-step QA
ai_capability_measured:
Scientific reasoning, deep knowledge

metrics: - Accuracy

models: - o1 - DeepSeek-R1

ml motif: - Reasoning & Generalization

type: Benchmark

ml task: - Supervised Learning

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

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

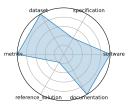
datasets.links.name: unknown
datasets.links.url: unknown
results.links.name: unknown
results.links.url: unknown
fair.reproducible: Yes
fair.benchmark ready: Yes

id: gpqa_diamond

Citations: [28]

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





3.45 PRM800K

PRM800K is a process supervision dataset containing 800,000 step-level correctness labels for model-generated solutions to problems from the MATH dataset.

date: 2023-05-30

version:

 last_updated:
 2023-05-30

 expired:
 false

 valid:
 yes

 valid date:
 2023-05-30

 ${\bf url:} \hspace{1.5cm} {\rm https://github.com/openai/prm800k/tree/main}$

doi: 10.48550/arXiv.2305.20050

domain: - 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: - GPT-4

ml motif: - Reasoning & Generalization

type: Benchmark ml task: - Reasoning

solutions: 0

notes: Math problems & Annotated reasoning steps based off of Dan Hendrycks' MATH dataset

contact.name: Karl Cobbe contact.email: karl@openai.com

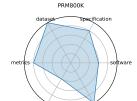
datasets.links.name: PRM800K: A Process Supervision Dataset datasets.links.url: https://github.com/openai/prm800k/tree/main

results.links.name: Let's Verify Step by Step

results.links.url: https://arxiv.org/abs/2305.20050

fair.reproducible: Yes
fair.benchmark_ready: Yes
id: prmk
Citations: [29]

Rating	Value	Reason
dataset	5	Dataset follows all FAIR Principles. Train/Test splits are available in the PRM800K repo
documentation	5	Documentation is present in the PRM800K repo and "Lets Verify Step by Step" paper.
metrics	4	Correctness is used as the primary metric, with grading guidelines provided.
reference_solution	2	A reference solution is mentioned in the "Lets Verify Step by Step" paper, but the model
		is not open-sourced.
software	3	Code is provided in the PRM800K Repo for evaluation and grading, documentation is
		present but no environment details, baseline model, or training code is given
specification	4	Task is well specified, format, inputs, and outputs are mentioned. No system constraints
		are provided.



3.46 FEABench (Finite Element Analysis Benchmark): Evaluating Language Models on Multiphysics Reasoning Ability

N/A

date: 2023-01-26

version: 1

 last_updated:
 2023-01-26

 expired:
 false

 valid:
 no

 valid date:
 2023-01-26

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

doi:unknowndomain:- Mathematics

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

licensing: unknown

task_types: - Simulation - Performance evaluation

ai capability measured: - Numerical simulation accuracy and efficiency

metrics:
- Solve time - Error norm
models:
- FEniCS - deal.II

ml motif: - Reasoning & Generalization

type: Benchmark

ml task: - Supervised Learning

solutions:unknownnotes:OKcontact.name:unknowncontact.email:unknown

datasets.links.name: FEABench Github

datasets.links.url: https://github.com/google/feabench?tab=readme-ov-file#datasets

results.links.name: unknown
results.links.url: unknown
fair.reproducible: Yes
fair.benchmark_ready: Yes

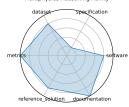
id: feabench_finite_element_analysis_benchmark_evaluating_language_models_on_multiphysics_reasoning_abi

Citations: [30]

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	Output is defined and task clarity is questionable

FEABench (Finite Element Analysis Benchmark): Evaluating Language Models on Multiphysics Reasoning Ability



3.47 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:
 - High Energy 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: - Classification 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: No

id: neural architecture codesign for fast physics applications

Citations: [31]

Ratings:

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
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

Neural Architecture Codesign for Fast Physics Applications



3.48 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:
 - 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

ml_motif: - Regression

type: Dataset + Benchmark

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.

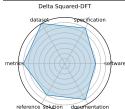
contact.name: Wei Liu
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: delta_squared-dft

Citations: [32]

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.



3.49 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/

 $\begin{array}{lll} \textbf{doi:} & 10.48550/\mathrm{arXiv.2503.02112} \\ \textbf{domain:} & - \text{Climate \& Earth Science} \\ \end{array}$

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
condels:
- CNNs, RNNs, Transformers

ml motif: - Anomaly Detection

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

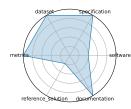
fair.reproducible: Yes fair.benchmark ready: Yes

id: hdr ml anomaly challenge - sea level rise

Citations: [33]

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.





3.50 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: - Biology & Medicine

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

 ${\bf models:} \qquad \quad - \ {\rm CNN\text{-}based} \ {\rm SSL} \ {\rm models}$

ml_motif: - Regression 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 Peterson
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark_ready: Yes

id: vocal call locator vcl

Citations: [34]

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.



3.51 MassSpecGym - De novo molecule generation

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

 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: unknowndomain: - Chemistry

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

 $ml_motif:$ - Generative

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

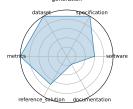
fair.reproducible: Yes fair.benchmark ready: Yes

id: massspecgym - de novo molecule generation

Citations: [35]

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.





3.52 MassSpecGym - Molecule Retrieval

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

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

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

doi: unknowndomain: - Chemistry

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

 $ml_motif:$ - Regression

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.

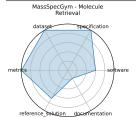
contact.name: Roman Bushuiev contact.email: unknown results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: massspecgym_-_molecule_retrieval

Citations: [35]

Rating	Value	Reason
dataset	5	Largest public MS/MS dataset with extensive annotations; minor point deducted for lack
1	-	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.



3.53 MassSpecGym - Spectrum Simulation

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

 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:unknowndomain:- Chemistry

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: - Regression

type: Dataset, Benchmark

ml task: - Generation, retrieval, simulation

solutions:

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

MS/MS tasks.

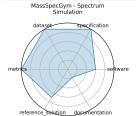
contact.name: Roman Bushuiev
contact.email: unknown
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: massspecgym_-_spectrum_simulation

Citations: [35]

Rating	Value	Reason
dataset	5	Largest public MS/MS dataset with extensive annotations; minor point deducted for lack
1	-	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.



3.54 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: - Computational Science & AI
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: - Multimodal Reasoning

type: Benchmark

ml task: - Supervised Learning

solutions: 0
notes: 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: Yes
fair.benchmark ready: Yes

id: spiqa_scientific_paper_image_question_answering

Citations: [36]

Rating	Value	Reason
dataset	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
${\tt reference_solution}$	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.





3.55 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: - Biology & Medicine - High Energy 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:
- Accuracy
models:
- GPT-4 baseline

ml motif: - Reasoning & Generalization

type: 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:unknowndatasets.links.name:GPQA datasetdatasets.links.url:zip/HuggingFaceresults.links.name:ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: gpqa_a_graduate-level_google-proof_question_and_answer_benchmark

Citations: [37]

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.





$3.56 \quad MedQA$

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:
 - Biology & Medicine

 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: - Reasoning & Generalization

type: Benchmark

ml task: - Supervised Learning

solutions: 0

notes: Multilingual (English, Simplified and Traditional Chinese)

contact.name: Di Jin

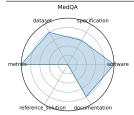
contact.email: jindi15@mit.edu

datasets.links.name: Github

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

results.links.name: unknown
results.links.url: unknown
fair.reproducible: Yes
fair.benchmark_ready: Yes
id: medqa
Citations: [38]

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.



3.57 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:
 - Computational Science & AI

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:
- Classification
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 datasetdatasets.links.url:zenodo.org/records/14427490

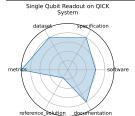
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: single_qubit_readout_on_qick_system

Citations: [39]

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.



3.58 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: - Mathematics

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: - Regression 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:Yesfair.benchmarkready:Yes

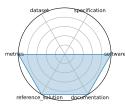
id: cfdbench_fluid_dynamics

Citations: [40]

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)



3.59 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: - Materials Science - High Energy Physics - Biology & Medicine - Chemistry - Climate & Earth

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

- Long-context understanding and scientific reasoning

- Multimodal comprehension

ai capability measured:

metrics: - Accuracy models: - unkown

ml motif: - Reasoning & Generalization

type: Benchmark

ml task: - Supervised Learning

solutions: 0 notes: Good

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: Yes
fair.benchmark ready: Yes

id: curie_scientific_long-context_understanding_reasoning_and_information_extraction

Citations: [41]

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)



3.60 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: - High Energy Physics

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:
- Classification
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

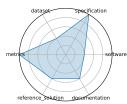
fair.reproducible: Yes

Citations: [42]

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
$reference_solution$	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



3.61 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

 $\mathbf{url:} \qquad \qquad \mathbf{https://arxiv.org/pdf/2107.02157}$

doi: unknown

domain: - High Energy Physics

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: - Anomaly Detection

 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 contact.email: ema.puljak@cern.ch

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

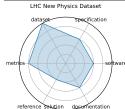
results.links.name: ChatGPT LLM

fair.reproducible: Yes fair.benchmark ready: Yes

id: lhc_new_physics_dataset

Citations: [43]

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.
LUC New Physics Dateset		1 / 1 V 1



3.62 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

url: https://github.com/XanaduAI/qml-benchmarks

 doi:
 10.48550/arXiv.2403.07059

 domain:
 - Computational Science & AI

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 probability
models:
- IBM Q - IonQ - AQT@LBNL

ml_motif: - Classification 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: Yes fair.benchmark ready: Yes

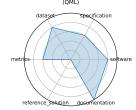
id: quantum_computing_benchmarks_qml

Citations: [44]

Ratings:

Rating	Value	Reason
dataset	4	Datasets are accessible, but not split.
documentation	5	Paper is available with all required information.
metrics	3	Partially defined, somewhat inferrable metrics. Unknown whether a system's performance is captured.
reference solution	0	Not provided
software	4	Software is built upon multiple common frameworks for simulation, training, and benchmarking workflows.
specification	3	No system constraints. Task clarity and dataset format are not clearly specified.

Quantum Computing Benchmarks (OML)



3.63 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

 url:
 https://arxiv.org/pdf/2402.01876

 doi:
 10.48550/arXiv.2402.01876

 domain:
 - High Energy 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:
metrics:
 - Real-time inference under FPGA constraints
 - Accuracy - Latency - Resource utilization
models:
 - MLP - Deep Sets - Interaction Network

ml motif: - Classification

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

 $\textbf{results.links.url:} \\ \text{https://docs.google.com/document/d/1gDf1CIYtfmfZ9urv1jCRZMYz_3WwEETkugUC65OZBdw} \\ \text{a.s.} \\ \text{ttps://docs.google.com/document/d/1gDf1CIYtfmfZ9urv1jCRZMYz_3WwEETkugUC65OZBdw} \\ \text{ttps://document/d/1gDf1CIYtfmfZ9urv1jCRZMYz_3WwEETkugUC65OZBdw} \\ \text{ttps://document/d/1gDf1CIYtfmfZ9urv1jCRZMYz_3WwEETkugUC65OZBdw}$

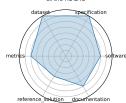
fair.reproducible: Yes fair.benchmark ready: No

id: ultrafast jet_classification_at_the_hl-lhc

Citations: [45]

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





3.64 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

 $\begin{array}{lll} \textbf{url:} & \text{https://arxiv.org/abs/2008.08198} \\ \textbf{doi:} & 10.48550/\text{arXiv.2008.08198} \end{array}$

domain: - Materials 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:
- Classification
type:
Framework
ml_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: Yes fair.benchmark ready: Yes

id: hedm braggnn

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
${\tt reference_solution}$	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





4D-STEM 3.65

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

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

doi: unknown

- Materials Science domain:

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

- CNN models (prototype) models:

ml motif: - Classification

Model type:

ml task: - Image Classification

solutions:

notes: In-progress; model design under development.

Shuyu Qin contact.name: contact.email: shq219@lehigh.edu results.links.name: ChatGPT LLM fair.reproducible: in progress fair.benchmark ready: No

id: $\operatorname{d-stem}$ Citations: [47]

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



3.66 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

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

 $\begin{array}{lll} \mbox{\bf doi:} & 10.48550/\mbox{arXiv}.2207.07958 \\ \mbox{\bf domain:} & -\mbox{High Energy Physics} \\ \end{array}$

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:
- Reinforcement Learning/Control

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: unknown
results.links.name: ChatGPT LLM
fair.reproducible: in progress
fair.benchmark_ready: in progress
id: beam_control
Citations: [48], [49]

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





3.67 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

 url:
 https://arxiv.org/pdf/2501.04845

 doi:
 10.48550/arXiv.2501.04845

 domain:
 - High Energy 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: - Classification

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

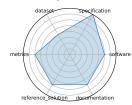
fair.reproducible: Yes fair.benchmark ready: No

id: intelligent_experiments_through_real-time_ai

Citations: [50]

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





3.68 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/

 $\begin{array}{lll} \textbf{doi:} & 10.48550/\mathrm{arXiv.2503.02112} \\ \textbf{domain:} & - \operatorname{Biology} \ \& \ \operatorname{Medicine} \\ \end{array}$

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 systems metrics: - Classification accuracy - F1 score

models: - CNN-based detectors
ml_motif: - Anomaly Detection

type: Dataset

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

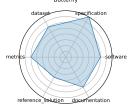
fair.reproducible: Yes fair.benchmark ready: Yes

id: hdr ml anomaly challenge - butterfly

Citations: [51]

Rating	Value	Reason
dataset	3	Dataset consists of real detector data with synthetic anomaly injections; access is restricted and requires NDA, limiting openness and FAIR compliance.
documentation	3	Challenge website provides basic descriptions and evaluation metrics but lacks comprehensive 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.





3.69 **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

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

 $\begin{array}{lll} \mbox{\bf doi:} & 10.48550/\mbox{arXiv.}2103.13910 \\ \mbox{\bf domain:} & -\mbox{High Energy Physics} \\ \end{array}$

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:
 - Anomaly Detection

 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

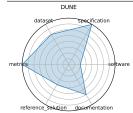
contact.name: Andrew J. Morgan

contact.email: unknown

datasets.links.name: DUNE SONIC data results.links.name: ChatGPT LLM

fair.reproducible: no fair.benchmark_ready: No dune Citations: [52]

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



3.70 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: - unknown

ml motif: - Reasoning & Generalization

type: Benchmark

ml task: - Supervised Learning

solutions: 0

notes: More information available at https://epoch.ai/frontiermath/about

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

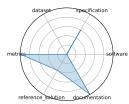
datasets.links.name:unknowndatasets.links.url:unknownresults.links.name:unknownresults.links.url:unknownfair.reproducible:Nofair.benchmarkready:No

id: frontiermath

Citations: [53]

Rating	Value	Reason
dataset	0	Only samples of dataset exist, not publicly available
documentation	5	All necessary information is in the paper and website
metrics	5	All questions in the dataset have a correct answer
$reference_solution$	2	Displays result of leading models on the benchmark, but none are trainable or list constraints
software	0	No publicaly available code to run the benchmark
specification	3	Well-specified process for asking questions and receiving answers. No software or hardware constraints





3.71 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: - unknown

ml motif: - Reasoning & Generalization

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

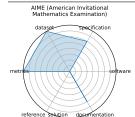
datasets.links.url: https://artofproblemsolving.com/wiki/index.php/AIME_Problems_and_Solutions

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

id: aime_american_invitational_mathematics_examination

Citations: [54]

Rating	Value	Reason
dataset	4	Easily accessible data with problems and solutions, but no splits
documentation	3	Some background and other information is provided, but it is not comprehensive. No info
		on how to run an evaluation
metrics	4	Correctness is measured, but no grading guidelines are provided.
reference solution	0	Not given. Human performance stats exist, but no mentions of AI performance
software	0	No code available
specification	3	Task and Inputs/Outputs are well specified. No system constraints or dataset format is
		mentioned



3.72 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: - High Energy Physics

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: - Anomaly Detection

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

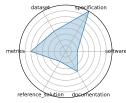
results.links.name: ChatGPT LLM fair.reproducible: in progress

fair.benchmark_ready: No id: No quench_detection

Citations: [55]

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





3.73 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: unknown

domain: - 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: - Regression 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

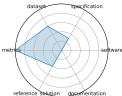
results.links.name: unknown
results.links.url: unknown
fair.reproducible: Yes
fair.benchmark ready: Yes

id: ____ materials_project

Citations: [56]

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.





3.74 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:
 - High Energy Physics

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:
 - Classification

 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: No

id: in-situ_high-speed_computer_vision

Citations: [57]

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



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