FAIR Surrogate Benchmarks Supporting AI and Simulation Research

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Open Source Web Sites

https://sbi-fair.github.io/docs/

https://github.com/mlcommons/science

OVERVIEW

The Surrogate Benchmark Initiative (SBI) project created a community repository and FAIR data ecosystem for HPC application surrogate benchmarks, including data, code, and all relevant collateral artifacts the science and engineering community needs to use and reuse these data sets and surrogates.

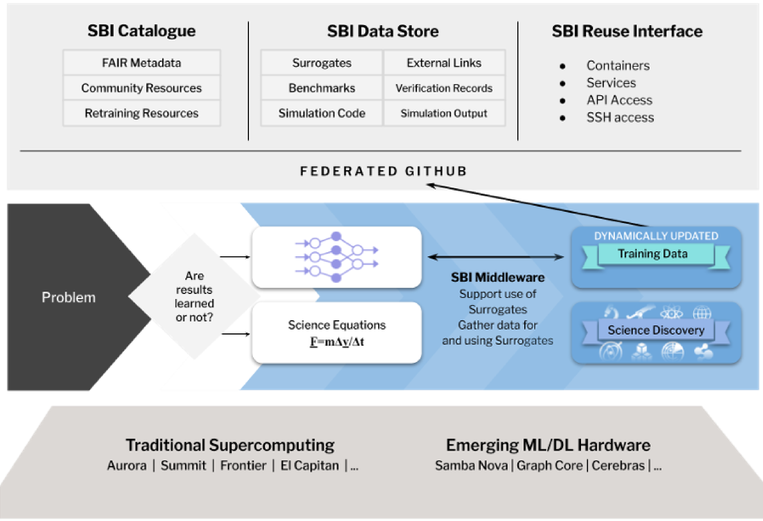
Application oriented benchmarks include:

- **AutoPhaseNN, Calorimeter, Virtual tissue, Cosmoflow. Ionized plasma. Ions in nanoconfinement, Molecule docking, miniWeatherML, OSMI, Particle dynamics, PtychoNN**

Software to promote FAIR include:

- **Sabath, Experiment Executor, and Compute Coordinator**

Very useful in Education.



FAIR Enabling Software

Sabbath specification

Compute Coordinator and Experiment Executor

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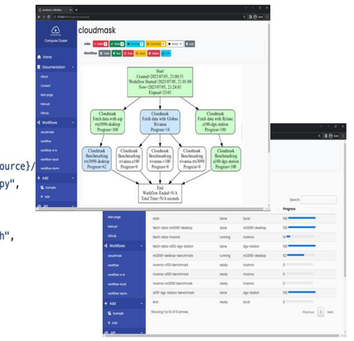
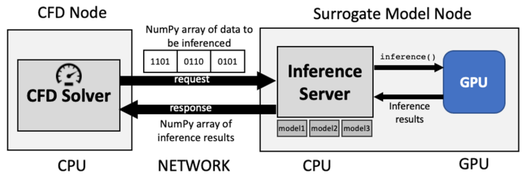
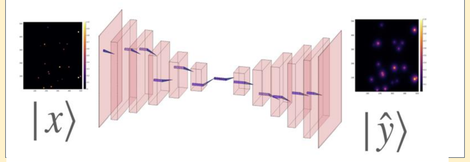


SBI Benchmark Applications

OSMI: Surrogate calculations via a Inference Server

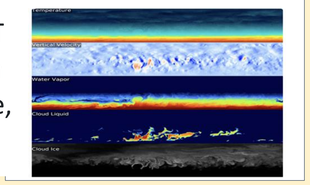


Virtual Tissue



Virtual tissue surrogate. Has three versions: 1) UNET for equilibrium, 2) Diffusion model for time dependence, 3) Digital Twin.

Mini-WeatherML

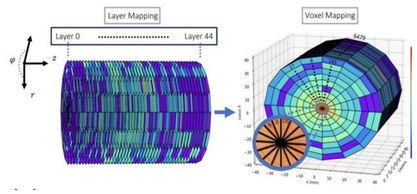


Kaggle Calorimeter Challenge

Uses generative AI to produce a surrogate for the Monte Carlo calculation of a calorimeter response (ATLAS data at LHC calculated with GEANT4).

Uniform benchmarking adding correlations

CaloDream **CaloDiffusion**
CaloScore **CaloINN**



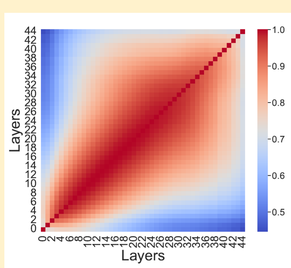
Calo4pQVAE: A Quantum-assisted 4 Partite VAE Calorimeter Surrogate

Fastest Calorimeter Surrogate developed with TRIUMF using Restricted Boltzmann Machines Annealed with **D-Wave Quantum Computer**

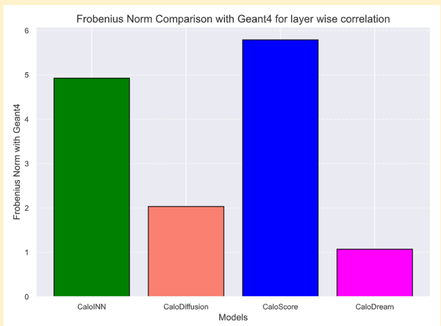
Model	Time per Shower ms	Energy per Shower Joule
GEANT	1000	8
CaloDream	74.3	30
CaloDiffusion	99.5	40
ConvL2LFlows	1.6	0.6
CaloScore (SS)	2.5	**1**
Calo4pQVAE	**0.181**	2
Annealing	0.020	0.3
Readout	0.087	1.6
Wait	0.020	0.3
GPU	0.054	<0.1

Can lower energy consumption of all surrogates using GPU reduced precision

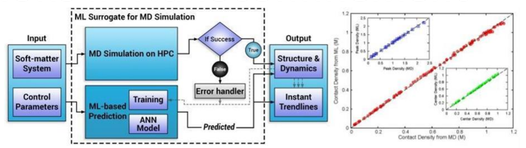
New Correlation Metrics to further compare the models . Exploring use of Correlation and Errors in training. Note error in energy E proportional to √E



Geant4

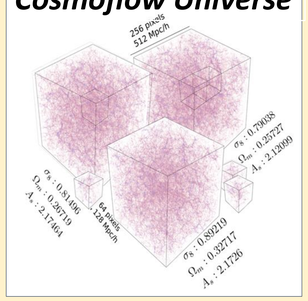


Ions in Nanoconfinement



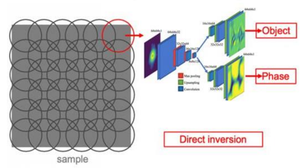
(left) Architecture of dynamic training of ML surrogate and (right) Comparison of three final state densities (peak, contact, and center) between MD simulations and NN surrogate predictions

Cosmoflow Universe

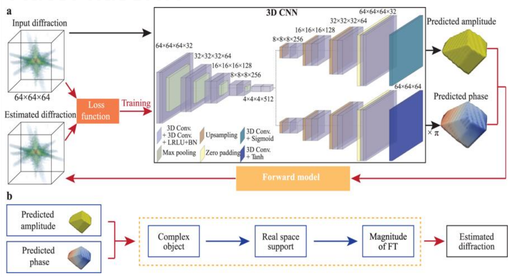


PtychoNN

learns to predict the sample amplitude and phase from nano-focused X-ray scanning data.

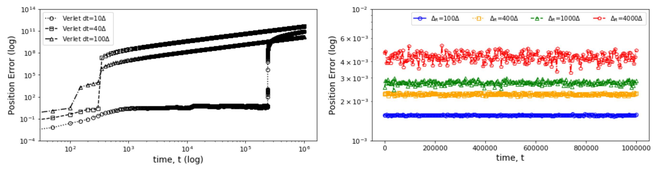


AutoPhaseNN



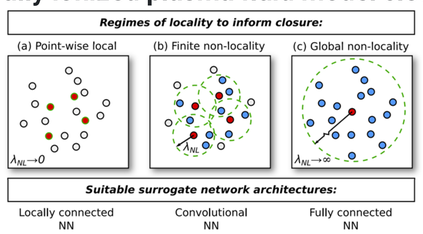
Unsupervised physics-aware deep learning of 3D nanoscale Bragg coherent diffraction imaging

MD: Molecular Dynamics



Recurrent Neural Nets as a Particle Dynamics Integrator. Average error in position updates for 16 particles interacting with an LJ potential, The left figure is standard MD with error increasing for Δt as 10, 40, or 100 times robust choice (0.001). On the right is the LSTM network with modest error up to t = 10^6 even for Δt = 4000 times the robust MD choice. x

Fully ionized plasma fluid model closure



The closure problem in fluid modeling is a well-known challenge to modelers aiming to accurately describe their system of interest.

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