Contribution ID: **29** Type: **not specified**

Machine-Learned Density of States in Multicanonical Simulations

Monday 1 December 2025 14:00 (40 minutes)

Since the density of states (DOS) is the foundation for our capacity to compute thermodynamic characteristics, sample complex energy landscapes, and describe rare-event behaviour, accurately calculating the DOS is a crucial challenge in many fields of computational physics. For applications like neutron spectrum analysis, surrogate modelling of reactor behaviour, and uncertainty quantification in research reactor simulations, accurate DOS estimation is becoming increasingly crucial in nuclear science. Nevertheless, DOS reconstruction is computationally costly and possibly imprecise since conventional Monte Carlo techniques frequently fail to sufficiently sample low-probability energy regions.

To get over these restrictions and enable effective, high-fidelity DOS estimation, we introduce in this work a hybrid multicanonical (MUCA) Monte Carlo–machine learning (ML) system. To create energy histograms with improved coverage of uncommon or otherwise challenging-to-sample areas of the energy domain, the procedure makes use of MUCA sampling. A neural surrogate model that learns a smooth, continuous, and differentiable approximation of the DOS is subsequently trained using these enhanced datasets. The ML-based DOS representation is incredibly quick to assess after training and may be applied to several reweighting jobs without
the need for more costly sampling.

We apply the approach to simpler neutron-energy-based models inspired by situations found in research reactor facilities to demonstrate its possibilities. The findings show that while significantly lowering the quantity of MUCA sampling needed, the ML assisted DOS estimator effectively replicates the qualitative characteristics and important structures of the genuine DOS. Additionally, the learnt DOS surrogate makes it possible to evaluate reweighted observables quickly and adaptably, which opens the door to effective parametric investigations and inverse analyses.

All things considered, this hybrid MUCA–ML approach offers a computationally effective basis for combining cutting-edge sampling techniques with contemporary learning methods in reactor simulation. The method has a wide range of potential applications in low-power, training-oriented research reactors and related nuclear systems, including enhancing spectral analysis workflows, speeding up surrogate generation, and assisting with uncertainty quantification and inverse problem-solving

Special requests

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Session Classification: Talks