Machine learning for physics simulation anomaly detection

Adam Good[a], Howard Pritchard[b], Lissa Moore[c], and Garrett Kenyon[d]

[a,b,c,d]Los Alamos National Laboratory, Los Alamos NM, USA

ABSTRACT

Multi-physics hydrodynamic direct numerical simulations (DNS) are often computationally intensive, requiring significant computational resources to complete. For simulations requiring thousands of processors, the proba- bility of anomalies occurring during a simulation is not insignificant. Since these simulations often run for a long time without human validation, such undetected anomalies can be costly. We present results of our application of ML based techniques for anomaly detection to hydrodynamics simulations. By treating the intermediate output of hydrodynamic simulations as images or videos, we borrow ML techniques from computer vision for the task of anomaly detection. We generated a training dataset using CLAMR, a cell-based adaptive mesh refinement application which implements the shallow water equations. Modifications were done to the application to obtain a wider range of experiments for our dataset. We generated a range of experiments who's states can be learned using computer vision techniques. Additionally, those same experiments could be run with anomalies injected at runtime so our models could be trained to differentiate between nominal and anomalous simulation states. We also present ML models using PetaVision, a neuromorphic computing simulation toolkit, as well as other autoencoders, and demonstrate that they can predict the state of a simulation at a succeeding time step based on the states of a number of preceding time steps. Additionally, we use these autoencoders with a classifier to determine if a given simulation state is anomalous. Our experiments show that out models can predict simulation state accurately enough for the classifier to detect anomalies despite notable differences between predictions.

LA-UR-21-27178